10/689,122

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[redacted]

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NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	AUG 09	INSPEC enhanced with 1898-1968 archive
NEWS 4	AUG 28	ADISCTI Reloaded and Enhanced
NEWS 5	AUG 30	CA(SM)/CAplus(SM) Austrian patent law changes
NEWS 6	SEP 21	CA/CAplus fields enhanced with simultaneous left and right truncation
NEWS 7	SEP 25	CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS 8	SEP 25	CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS 9	SEP 25	CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS 10	SEP 28	CEABA-VTB classification code fields reloaded with new classification scheme
NEWS 11	OCT 19	LOGOFF HOLD duration extended to 120 minutes
NEWS 12	OCT 19	E-mail format enhanced
NEWS 13	OCT 23	Option to turn off MARPAT highlighting enhancements available
NEWS 14	OCT 23	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 15	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS 16	OCT 30	CHEMLIST enhanced with new search and display field
NEWS 17	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS 18	NOV 10	CA/CAplus F-Term thesaurus enhanced
NEWS 19	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS 20	NOV 20	CAS Registry Number crossover limit increased to 300,000 in additional databases
NEWS 21	NOV 20	CA/CAplus to MARPAT accession number crossover limit increased to 50,000
NEWS 22	DEC 01	CAS REGISTRY updated with new ambiguity codes
NEWS 23	DEC 11	CAS REGISTRY chemical nomenclature enhanced
NEWS 24	DEC 14	WPIDS/WPINDEX/WPIX manual codes updated
NEWS 25	DEC 14	GBFULL and FRFULL enhanced with IPC 8 features and functionality
NEWS 26	DEC 18	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS 27	DEC 18	CA/CAplus patent kind codes updated
NEWS 28	DEC 18	MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS 29	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS 30	DEC 27	CA/CAplus enhanced with more pre-1907 records

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items

```
 NEWS IPC8      For general information regarding STN implementation of IPC 8
 NEWS X25       X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that
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FILE 'HOME' ENTERED AT 16:59:57 ON 03 JAN 2007

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files.  For example, the EXPAND
command can only be used to look at the index in a file which has an
index.  Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of
commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                    0.21       0.21

FILE 'REGISTRY' ENTERED AT 17:00:12 ON 03 JAN 2007
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STRUCTURE FILE UPDATES:     2 JAN 2007  HIGHEST RN 916646-22-5
DICTIONARY FILE UPDATES:    2 JAN 2007  HIGHEST RN 916646-22-5

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

  Please note that search-term pricing does apply when
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experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10689122.str
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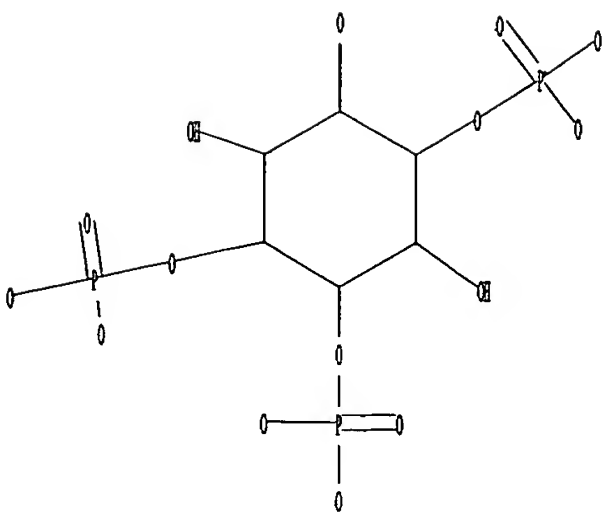
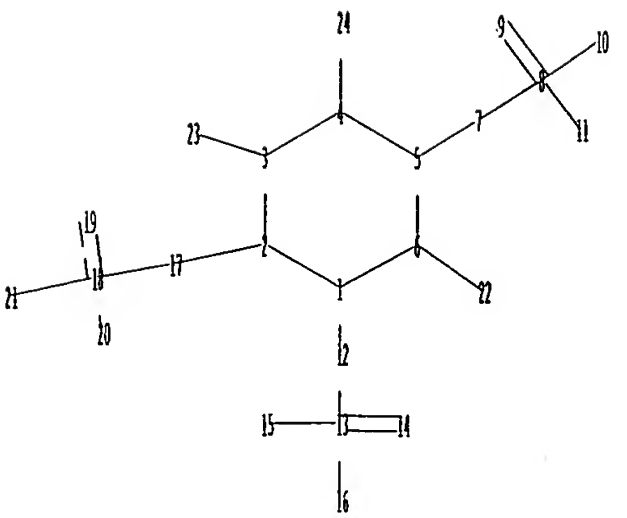


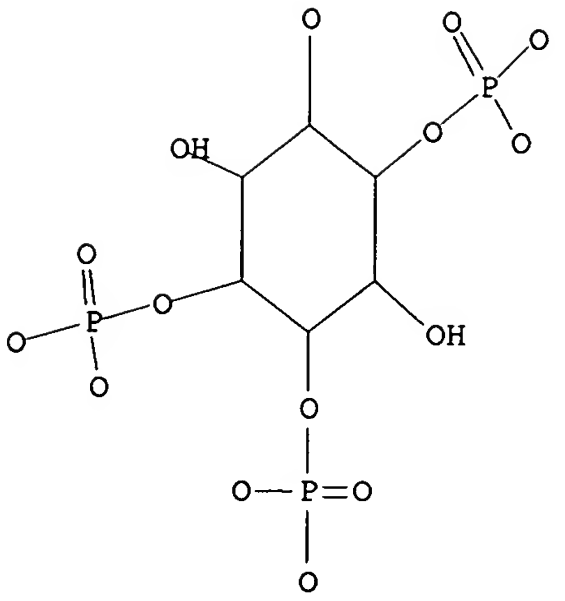


chain nodes :
7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
ring nodes :
1 2 3 4 5 6
chain bonds :
1-12 2-17 3-23 4-24 5-7 6-22 7-8 8-9 8-10 8-11 12-13 13-14 13-15 13-16
17-18 18-19 18-20 18-21
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-12 2-17 3-23 4-24 5-7 6-22 7-8 8-9 8-10 8-11 12-13 13-14 13-15 13-16
17-18 18-19 18-20 18-21
exact bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS 22:Atom 23:Atom 24:Atom

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

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=> s l1
SAMPLE SEARCH INITIATED 17:00:29 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      175 TO ITERATE

100.0% PROCESSED      175 ITERATIONS                          20 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          2707 TO     4293
PROJECTED ANSWERS:              132 TO      668

L2            20 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 17:00:38 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     3957 TO ITERATE

100.0% PROCESSED     3957 ITERATIONS                         445 ANSWERS
SEARCH TIME: 00.00.01

L3           445 SEA SSS FUL L1

=> FIL CAPLUS
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                               ENTRY    SESSION
FULL ESTIMATED COST                           172.10     172.31

FILE 'CAPLUS' ENTERED AT 17:00:43 ON 03 JAN 2007
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FILE COVERS 1907 - 3 Jan 2007 VOL 146 ISS 2
FILE LAST UPDATED: 2 Jan 2007 (20070102/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

```
=> s l3
L4          7495 L3

=> s l4 and (conjugate or label or tracer)
           67258 CONJUGATE
           60273 CONJUGATES
          104525 CONJUGATE
                 (CONJUGATE OR CONJUGATES)
           63086 LABEL
           21921 LABELS
           75861 LABEL
                 (LABEL OR LABELS)
           54936 TRACER
           19021 TRACERS
           64953 TRACER
                 (TRACER OR TRACERS)
L5           105 L4 AND (CONJUGATE OR LABEL OR TRACER)

=> s l5 and IP3R or IP3 receptor
            559 IP3R
           5376 IP3
         681077 RECEPTOR
         624756 RECEPTORS
         810862 RECEPTOR
                (RECEPTOR OR RECEPTORS)
           1251 IP3 RECEPTOR
                (IP3(W)RECEPTOR)
L6         1254 L5 AND IP3R OR IP3 RECEPTOR

=> s l5 and (IP3R or IP3 receptor)
            559 IP3R
           5376 IP3
         681077 RECEPTOR
         624756 RECEPTORS
         810862 RECEPTOR
                (RECEPTOR OR RECEPTORS)
           1251 IP3 RECEPTOR
                (IP3(W)RECEPTOR)
L7           14 L5 AND (IP3R OR IP3 RECEPTOR)

=> d l7 ibib abs hitstr tot

L7   ANSWER 1 OF 14  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2004:371146  CAPLUS
DOCUMENT NUMBER:          140:371475
TITLE:                    IP3 protein binding assay using detectably-labeled IP3
                          and an extracellular fragment of the IP3
                          receptor as reagents
INVENTOR(S):              Naqvi, Tabassum; Rouhani, Riaz; Fung, Peter; Eglen,
                          Richard; Singh, Rajendra
PATENT ASSIGNEE(S):       Discoverx, Inc., USA
```

inventors/

SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004038369	A2	20040506	WO 2003-US33262	20031020
WO 2004038369	A3	20040701		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2503228	A1	20040506	CA 2003-2503228	20031020
AU 2003301583	A1	20040513	AU 2003-301583	20031020
US 2004106158	A1	20040603	US 2003-689122	20031020
EP 1556682	A2	20050727	EP 2003-809590	20031020
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006503582	T	20060202	JP 2004-546937	20031020
PRIORITY APPLN. INFO.:			US 2002-420469P P	20021021
			WO 2003-US33262 W	20031020

Priority

OTHER SOURCE(S): MARPAT 140:371475

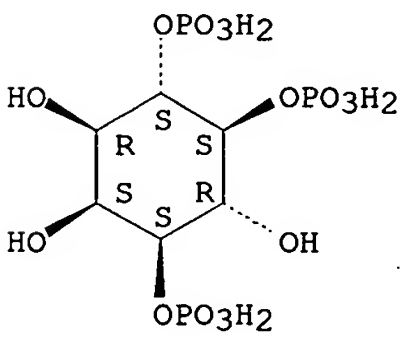
AB Protein binding assays are provided for determining IP3 in a sample employing as reagents a conjugate of IP3 joined at the 2-oxy through a bond or linking group to a detectable label and a truncated portion of the extracellular fragment of an IP3R. The reagents are combined with the sample and the amount of IP3 determined by means of the detectable label. The conjugate with the enzyme donor fragment of β-galactosidase or a fluorescer is specifically described.

IT 2068-89-5
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(IP3 protein binding assay using detectably-labeled IP3 and IP3 receptor extracellular fragment as reagents)

RN 2068-89-5 CAPLUS

CN D-myo-Inositol, 3,5,6-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



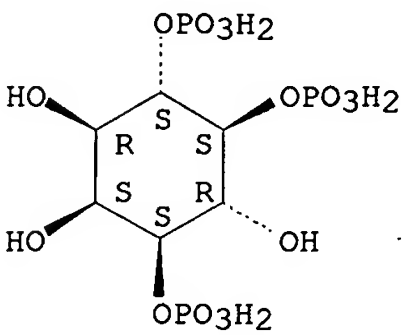
IT 2068-89-5D, conjugates with detectable label
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);

ANST (Analytical study); BIOL (Biological study); USES (Uses)
(IP3 protein binding assay using detectably-labeled IP3 and IP3 receptor extracellular fragment as reagents)

RN 2068-89-5 CAPLUS

CN D-myo-Inositol, 3,5,6-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

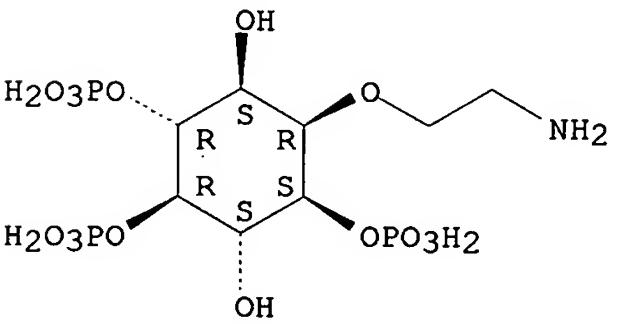


IT 502159-32-2DP, reaction product with hexachlorofluorescein N-hydroxysuccinimide derivative 685515-03-1DP, conjugates with β-galactosidase fragment 685515-04-2P 685515-07-5P 685515-08-6P
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)
(IP3 protein binding assay using detectably-labeled IP3 and IP3 receptor extracellular fragment as reagents)

RN 502159-32-2 CAPLUS

CN D-myo-Inositol, 2-O-(2-aminoethyl)-, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

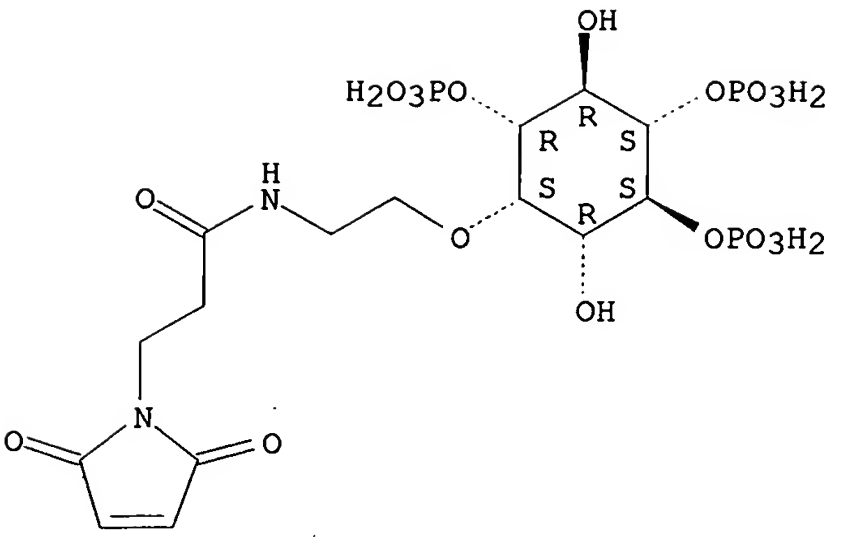
Absolute stereochemistry.



RN 685515-03-1 CAPLUS

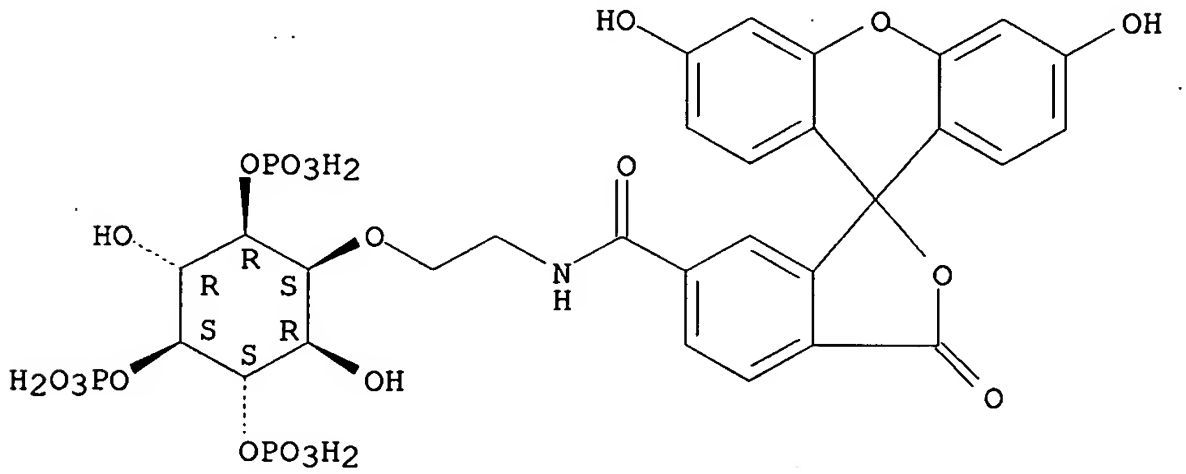
CN D-myo-Inositol, 2-O-[2-[[3-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxopropyl]amino]ethyl]-, 3,5,6-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



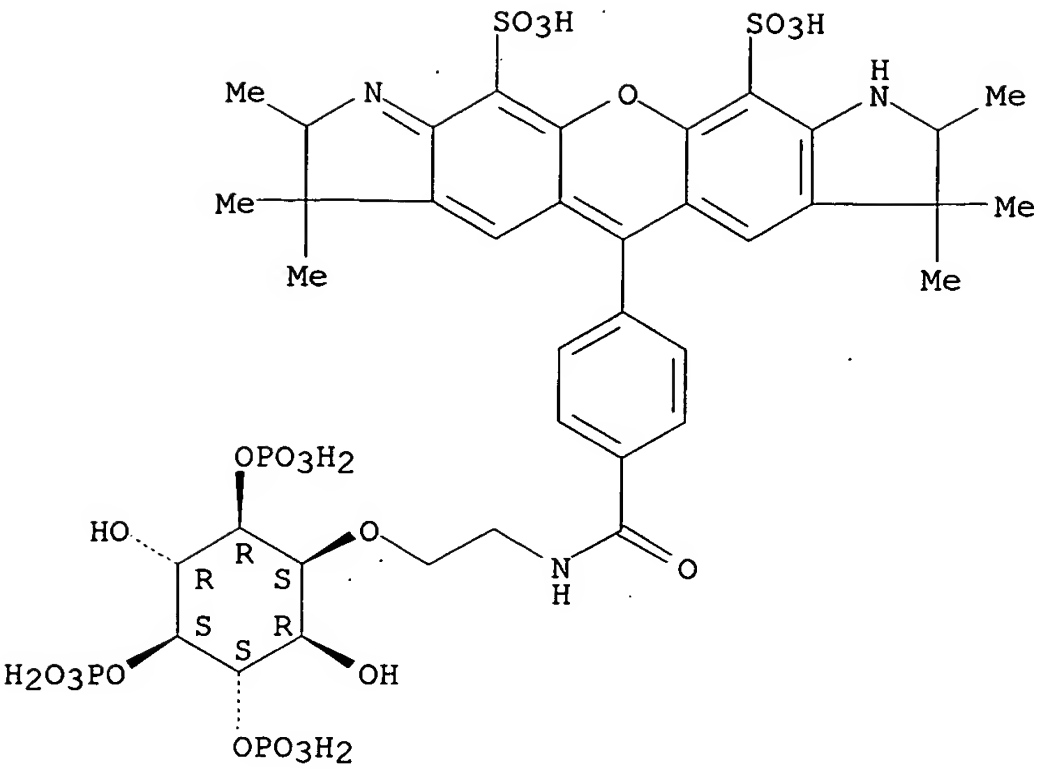
RN 685515-04-2 CAPLUS
CN D-myo-Inositol, 2-O-[2-[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl)carbonyl]amino]ethyl]-, 3,5,6-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 685515-07-5 CAPLUS
CN D-myo-Inositol, 2-O-[2-[[4-(2,3,7,8-tetrahydro-2,3,3,7,7,8-hexamethyl-10,12-disulfo-1H-pyrano[3,2-f:5,6-f']diindol-5-yl)benzoyl]amino]ethyl]-, 3,5,6-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

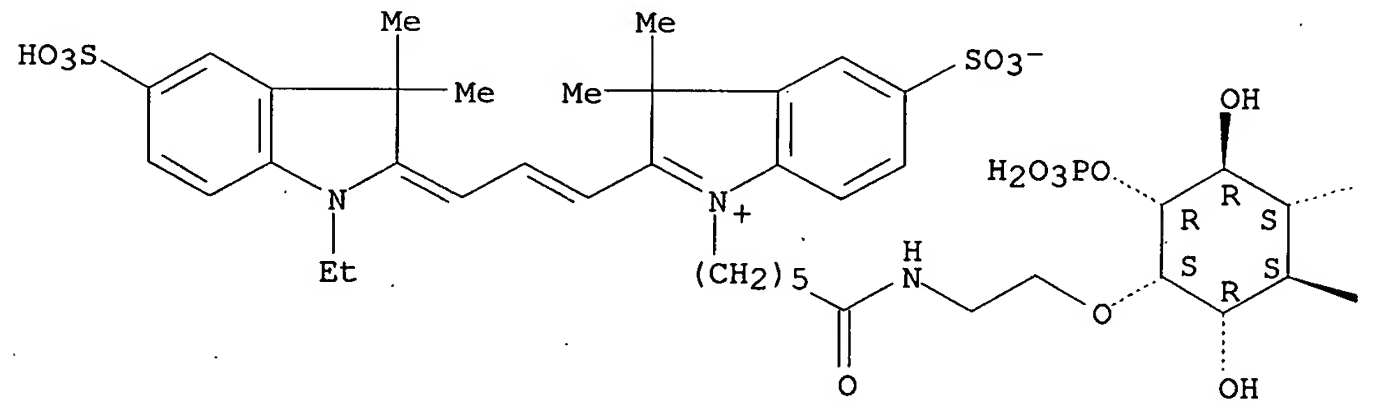
Absolute stereochemistry.



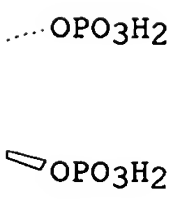
RN 685515-08-6 CAPLUS
CN D-myo-Inositol, 2-O-[2-[[6-[2-[3-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)-1-propenyl]-3,3-dimethyl-5-sulfo-3H-indolio]-1-oxohexyl]amino]ethyl]-, inner salt, 3,5,6-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



PAGE 1-B



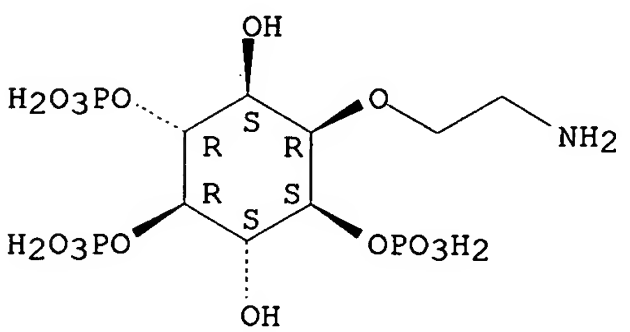
IT 502159-32-2 685515-06-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(IP3 protein binding assay using detectably-labeled IP3 and IP3

receptor extracellular fragment as reagents)

RN 502159-32-2 CAPLUS

CN D-myo-Inositol, 2-O-(2-aminoethyl)-, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 685515-06-4 CAPLUS

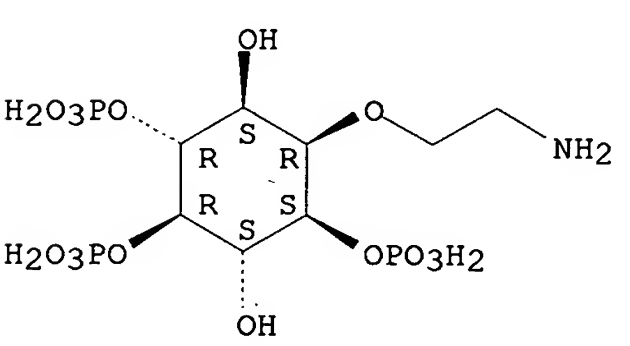
CN D-myo-Inositol, 2-O-(2-aminoethyl)-, 1,4,5-tris(dihydrogen phosphate), compd. with N,N-diethylethanamine (9CI) (CA INDEX NAME)

CM 1

CRN 502159-32-2

CMF C8 H20 N O15 P3

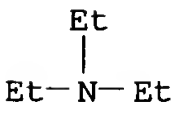
Absolute stereochemistry.



CM 2

CRN 121-44-8

CMF C6 H15 N



IT 685515-03-1P

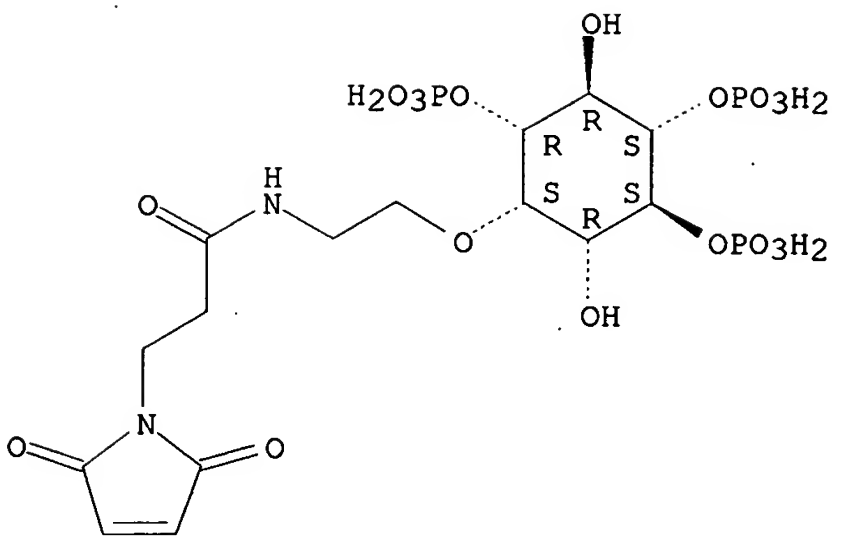
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(IP3 protein binding assay using detectably-labeled IP3 and IP3 receptor extracellular fragment as reagents)

RN 685515-03-1 CAPLUS

CN D-myo-Inositol, 2-O-[2-[[3-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxopropyl]amino]ethyl]-, 3,5,6-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



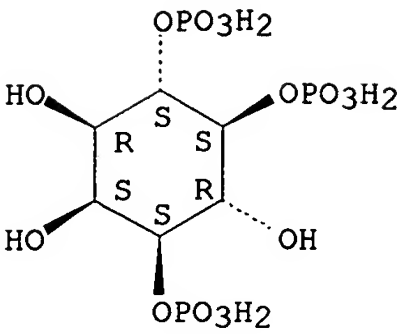
L7 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:500894 CAPLUS
DOCUMENT NUMBER: 140:402583
TITLE: Spatiotemporal Laser Inactivation of Inositol 1,4,5-Trisphosphate Receptors Using Synthetic Small-Molecule Probes
AUTHOR(S): Inoue, Takanari; Kikuchi, Kazuya; Hirose, Kenzo; Iino, Masamitsu; Nagano, Tetsuo
CORPORATE SOURCE: Graduate School of Medicine, Graduate School of Pharmaceutical Sciences, The University of Tokyo, Bunkyo-ku, Tokyo, 113-0033, Japan
SOURCE: Chemistry & Biology (2003), 10(6), 503-509
CODEN: CBOLE2; ISSN: 1074-5521
PUBLISHER: Cell Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A malachite green-conjugated inositol 1,4,5-trisphosphate (MGIP3) induces specific inactivation of IP3 receptor (IP3R) in tissue samples upon laser irradiation To verify potential usefulness of the method for studies of cellular Ca2+ signaling, we conducted laser inactivation at the single-cell level and show that IP3R was inactivated with extremely high spatiotemporal resolution In the presence of MGIP3, the Ca2+ release function of IP3R in single B lymphoma cells decayed exponentially with increasing duration of laser irradiation with a time constant of 3.4 s. Moreover, by confining laser irradiation to a spatially distinct region of differentiated PC12 cells, subcellular inactivation of IP3R was attained, as revealed by a loss of local Ca2+ signal. Such real-time inactivation of IP3R only within a subcellular region may provide a powerful method for investigating spatiotemporal dynamics of Ca2+ signaling.

IT 88269-39-0D, Inositol-1,4,5-trisphosphate, malachite green-conjugates
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(malachite green-conjugated inositol 1,4,5-trisphosphate-mediated laser inactivation of inositol 1,4,5-trisphosphate receptors in relation to calcium signaling studies)

RN 88269-39-0 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

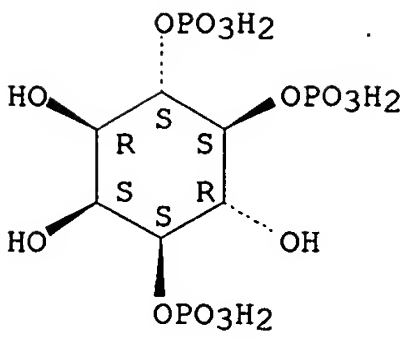
Relative stereochemistry.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:307779 CAPLUS
DOCUMENT NUMBER: 135:91476
TITLE: Control of Ca2+ influx in human neutrophils by inositol 1,4,5-trisphosphate (IP3) binding: differential effects of micro-injected IP3 receptor antagonists
AUTHOR(S): Davies-Cox, Eryl V.; Laffafian, Iraj; Hallett, Maurice B.
CORPORATE SOURCE: Molecular Signalling Group, University Department of Surgery, University of Wales College of Medicine, Cardiff, CF4 4XN, UK
SOURCE: Biochemical Journal (2001), 355(1), 139-143
CODEN: BIJOAK; ISSN: 0264-6021
PUBLISHER: Portland Press Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Neutrophils signal Ca2+ changes in response to occupancy of G-protein-linked receptors such as the formylated peptide receptor. This Ca2+ signal is composed of 2 parts, inositol 1,4,5-trisphosphate (IP3)-triggered release of Ca2+ from an intracellular store and Ca2+ influx. In order to probe the relation between these events, cytosolic free Ca2+ changes in neutrophils were monitored after micro-injection of agents which inhibit IP3 binding. Micro-injection of heparin into neutrophils totally inhibited both formyl-Met-Leu-Phe-induced Ca2+ release and the subsequent Ca2+ influx. This effect was not due to prior depletion of Ca2+ stores. Furthermore, micro-injection with anti-IP3-receptor antibody also inhibited Ca2+ release. However, anti-IP3-receptor antibody and another high-mol.-mass IP3-binding antagonist, heparin-albumin conjugate , failed to inhibit the accompanying Ca2+ influx. Thus, 2 IP3-binding sites exist in neutrophils: one accessible by both heparin and the high-mol.-mass inhibitors of IP3 binding and responsible for Ca2+ release, and another inaccessible to high-mol.-mass mols. and responsible for Ca2+ influx.
IT 88269-39-0, Inositol 1,4,5-trisphosphate
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(calcium influx in human neutrophils control by inositol 1,4,5-trisphosphate (IP3) binding in relation to IP3 receptor expression)
RN 88269-39-0 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Relative stereochemistry.



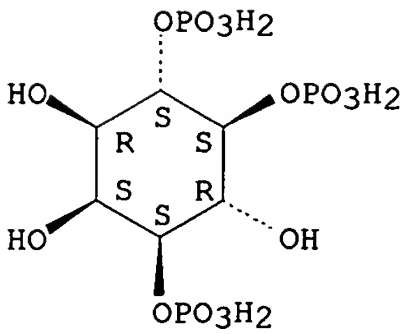
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:113310 CAPLUS
DOCUMENT NUMBER: 134:188476
TITLE: Inositol 1,4,5-trisphosphate receptor isoform expression in mouse pancreatic islets: effects of carbachol
AUTHOR(S): Lee, B.; Laychock, S. G.
CORPORATE SOURCE: Department of Pharmacology and Toxicology, State University of New York at Buffalo, School of Medicine and Biomedical Sciences, Buffalo, NY, 14214, USA
SOURCE: Biochemical Pharmacology (2001), 61(3), 327-336
CODEN: BCPCA6; ISSN: 0006-2952
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The inositol 1,4,5-trisphosphate receptors (IP3Rs) are ligand-gated Ca2+ channels that regulate intracellular Ca2+ mobilization. Among the IP3R mRNA isoforms I, II, and III, IP3R-I mRNA was expressed in mouse islets and the β-cell line βTC3, and was quant. the most abundant isoform as determined by reverse transcriptase-polymerase chain reaction. IP3R-II and -III mRNAs were expressed at similar levels in mouse islets, but neither isoform was detected in βTC3 cells. Culture of mouse islets for 30 min and 2 h at 20 mM glucose, or for 7 days at 11 mM glucose did not affect IP3R-I mRNA expression compared with islets cultured in 5.5 mM glucose. Culture of islets or βTC3 cells with carbachol (0.5 mM) reduced IP3R-I mRNA expression levels below control. Mouse islet α- and β-cells expressed IP3R-I and -III proteins, but IP3R-II protein was not detected by immunoblot or double-label immunohistochem. Culture of islets for up to 6 h with carbachol reduced IP3R-I and -III protein expression in a time-dependent manner with a half-maximal effect on type I at 1 h. Glucose (20 mM) stimulation for 2 h did not affect IP3R-1 levels. The carbachol-induced decrease in IP3R-I and -III protein expression was reversed by MG-132, a proteasome inhibitor. Thus, glucose failed to regulate mouse islet IP3R mRNA expression, whereas carbachol stimulation down-regulated IP3R mRNA and protein. A proteasomal protein degradative pathway appeared to mediate the muscarinic receptor-induced effects on IP3R-I and -III.

IT 88269-39-0, Inositol 1,4,5-trisphosphate
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(carbachol down-regulation of inositol trisphosphate receptor isoform expression in mouse pancreatic islets and β-cell line βTC3)
RN 88269-39-0 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Relative stereochemistry.



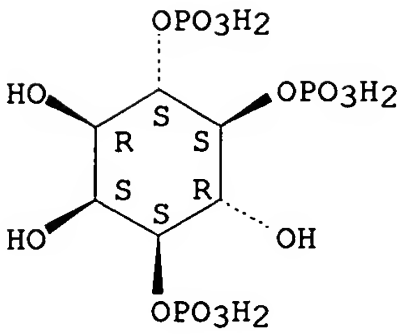
REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:491098 CAPLUS
DOCUMENT NUMBER: 133:173582
TITLE: Differential modulation of inositol 1,4,5-trisphosphate receptor type 1 and type 3 by ATP
AUTHOR(S): Maes, K.; Missiaen, L.; De Smet, P.; Vanlingen, S.; Callewaert, G.; Parys, J. B.; De Smedt, H.
CORPORATE SOURCE: Laboratorium voor Fysiologie, K U Leuven, Louvain, B-3000, Belg.
SOURCE: Cell Calcium (2000), 27(5), 257-267
CODEN: CECADV; ISSN: 0143-4160
PUBLISHER: Harcourt Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Binding of ATP to the inositol 1,4,5-trisphosphate receptor (IP3R) results in a more pronounced Ca2+ release in the presence of inositol 1,4,5-trisphosphate (IP3). Two recently published studies demonstrated a different ATP sensitivity of IP3-induced Ca2- release in cell types expressing different IP3R isoforms. Cell types expressing mainly IP3R3 were less sensitive to ATP than cell types expressing mainly IP3R1. To investigate the difference in ATP sensitivity between IP3R isoforms at the mol. level, microsomes of Sf9 insect cells expressing full-size IP3R1 or IP3R3 were covalently labeled with ATP by using the photoaffinity label 8-azido[α-32P]ATP. ATP labeling of the IP3R was measured after immunopptn. of IP3Rs with isoform-specific antibodies, SDS-PAGE and Phosphorimaging. Unlabeled ATP inhibited covalent linking of 8-azido[α-32P]ATP to the recombinant IP3R1 and IP3R3 with an IC50 of 1.6 μM and 177 μM, resp. MgATP was as effective as ATP in displacing 8-azido[α-32P]ATP from the ATP-binding sites on IP3R1 and IP3R3, and in stimulating IP3-induced Ca2+ release from permeabilized A7r5 and 16HBE14o- cells. The interaction of ATP with the ATP-binding sites on IP3R1 and IP3R3 was different from its interaction with the IP3-binding domains, since ATP inhibited IP3 binding to the N-terminal 581 amino acids of IP3R1 and IP3R3 with an IC50 of 353 μM and 4.0 mM, resp. The ATP-binding sites of IP3R1 bound much better ATP than ADP, AMP and particularly GTP, while IP3R3 displayed a much broader nucleotide specificity. These results therefore provide mol. evidence for a differential regulation of IP3R1 and IP3R3 by ATP.

IT 88269-39-0, Inositol-1,4,5-trisphosphate
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(differential modulation of inositol 1,4,5-trisphosphate receptor type 1 and type 3 by ATP)
RN 88269-39-0 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Relative stereochemistry.



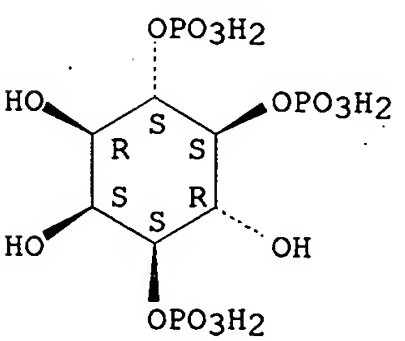
REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:605124 CAPLUS
DOCUMENT NUMBER: 127:261682
TITLE: Localization of a putative inositol 1,4,5-triphosphate receptor in the Limulus granulocyte
AUTHOR(S): Solon, Eric; Gupta, Ayodhya P.; Gaugler, Randy
CORPORATE SOURCE: Schering-Plough Research Institute, Kenilworth, NJ, 07033-0539, USA
SOURCE: Developmental and Comparative Immunology (1997), 21(3), 277-285
CODEN: DCIMDQ; ISSN: 0145-305X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The horseshoe crab (Limulus polyphemus) granulocyte (GR) degranulates upon contact with bacteria and factors are released that mediate an immune response. Stimulated cells produce IP3, which binds to receptors (IP3R, mol. weight 240-300 kDa) that function to release stored Ca2+ into the cytoplasm that mediates degranulation. This mechanism is believed to mediate exocytosis in the Limulus GR but IP3R in the GR has not been shown. The present study utilized monoclonal antibody 4C11 and a com. available anti-IP3R antibody, both of which label amino acids of the N-terminal of all known isoforms. Electron microscopy, immunohistochem., SDS-PAGE, and Western blot anal., which employed the use of the two antibodies, demonstrated that a putative IP3R exists in the: plasma membrane, smooth surfaced vesicles, nucleus, and nuclear membrane. The authors hypothesize that this putative IP3R is involved in mediating the immune response of the Limulus GR.

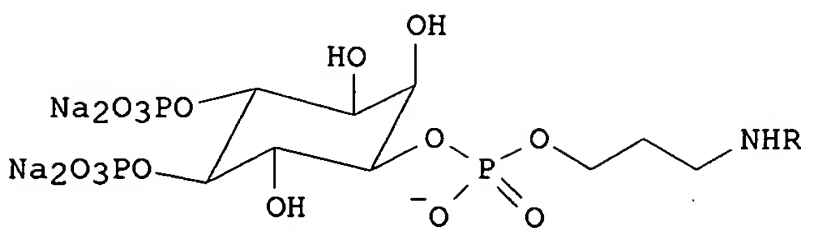
IT 88269-39-0, Inositol 1,4,5-triphosphate
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(receptor; inositol 1,4,5-triphosphate receptor localization in horseshoe crab granulocytes)
RN 88269-39-0 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:968820 CAPLUS
DOCUMENT NUMBER: 124:176713
TITLE: Synthesis of D-myo-P-1-(O-aminopropyl)-inositol-1,4,5-trisphosphate affinity probes from α-D-glucose
AUTHOR(S): Dorman, Gyorgy; Chen, Jian; Prestwich, Glenn D.
CORPORATE SOURCE: Dep. Chem., Univ. Stony Brook, Stony Brook, NY, 11794-3400, USA
SOURCE: Tetrahedron Letters (1995), 36(48), 8719-22
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:176713
GI



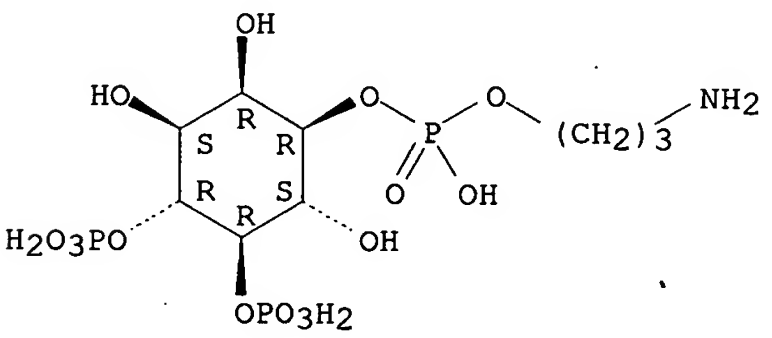
I

AB D-Myo-P1-(O-3-aminopropyl)-ins(1,4,5)P3 (I; R = H)(II) was synthesized from Me α-D-glucopyranoside via the Ferrier rearrangement. II was converted to the 4-benzoyldihydrocinnamoyl derivative (I; R = COCH2CH2C6H4Bz-4), a selective photoaffinity label for modification of the ligand binding site of IP3 receptor proteins.

IT 173831-00-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of P-(aminopropyl) D-myo-inositol trisphosphate (IP3) affinity probes)

RN 173831-00-0 CAPLUS
CN D-myo-Inositol, 1-(3-aminopropyl hydrogen phosphate) 4,5-bis(dihydrogen phosphate), tetrasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●4 Na

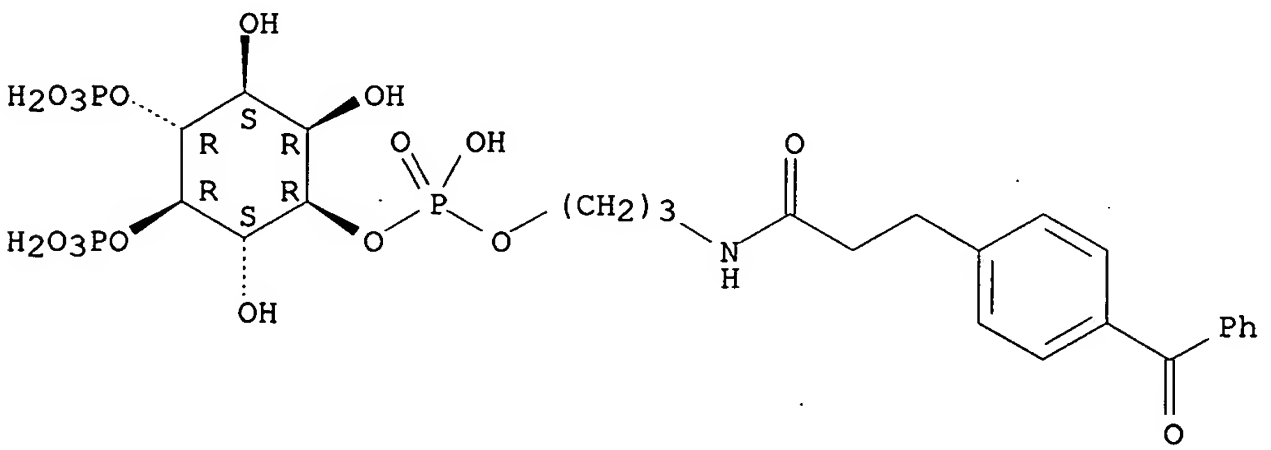
IT 173831-01-1P 173831-02-2P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of P-(aminopropyl) D-myo-inositol trisphosphate (IP3) affinity probes)

RN 173831-01-1 CAPLUS

CN D-myo-Inositol, 1-[3-[[3-(4-benzoylphenyl)-1-oxopropyl]amino]propyl hydrogen phosphate] 4,5-bis(dihydrogen phosphate), tetrasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

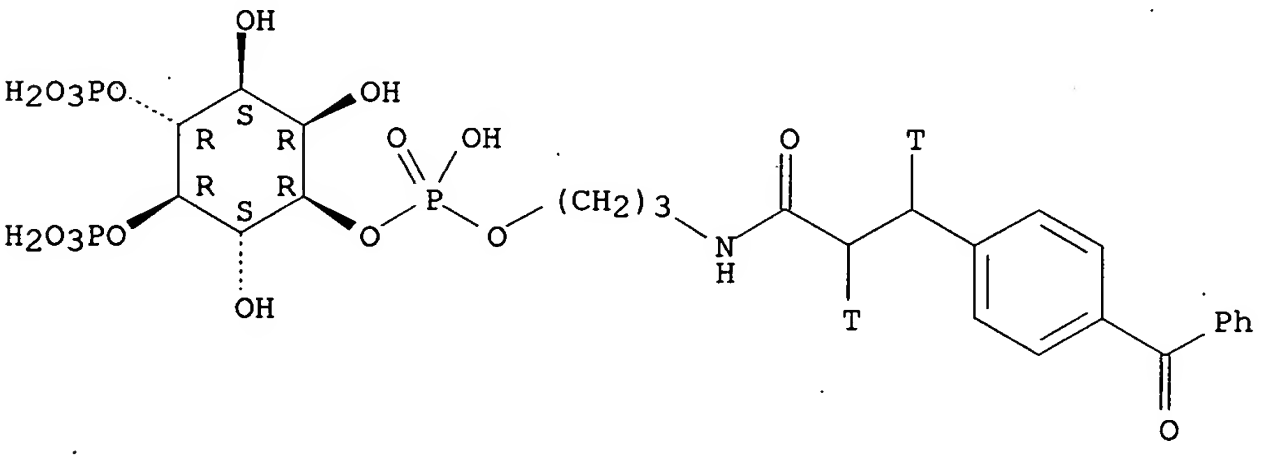


●4 Na

RN 173831-02-2 CAPLUS

CN D-myo-Inositol, 1-[3-[[3-(4-benzoylphenyl)-1-oxopropyl-2,3-t2]amino]propyl hydrogen phosphate] 4,5-bis(dihydrogen phosphate), tetrasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●4 Na

L7 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:797922 CAPLUS

DOCUMENT NUMBER: 123:252247

TITLE: Inositol 1,4,5-trisphosphate receptors: Immunocytochemical localization in the dorsal cochlear nucleus

AUTHOR(S): Ryugo, D. K.; Pongstaporn, T.; Wright, D. D.; Sharp, A. H.

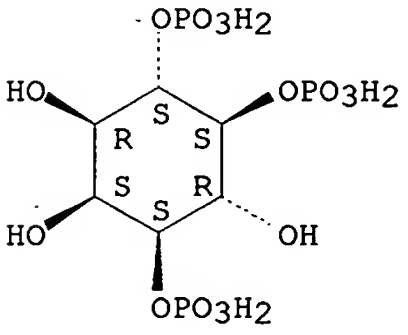
CORPORATE SOURCE: School Medicine, Johns Hopkins University, Baltimore, MD, 21205, USA

SOURCE: Journal of Comparative Neurology (1995), 358(1), 102-18
CODEN: JCNEAM; ISSN: 0021-9967
PUBLISHER: Wiley-Liss
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In the cochlear nucleus of mammals, the relatively homogeneous responses of auditory nerve fibers are transformed into a variety of different response patterns by the different classes of resident neurons. The spectrum of these responses is hypothesized to depend on the types and distribution of receptors, ion channels, G proteins, and second messengers that form the signaling capabilities in each cell class. In the present study, the authors examined the immunocytochem. distribution of the inositol 1,4,5-trisphosphate (IP3) receptor in the dorsal cochlear nucleus to better understand how this second messenger might be involved in shaping the neural signals evoked by sound. Affinity-purified polyclonal antibodies directed against the IP3 receptor labeled a homogeneous population of neurons in the dorsal cochlear nucleus of rats, guinea pigs, mustache bats, cats, New World owl monkey s, rhesus monkeys, and humans. These cells were all darkly immunostained except in the human where the labeling was less intense. Immunoblots of dorsal cochlear nucleus tissue from the rat revealed a single band of protein of mol. weight .apprx.260 kDa, which is the same size as the purified receptor, indicating that the antibodies reacted specifically with the IP3 receptor. These immunolabeled neurons were identified as cartwheel cells on the basis of shared characteristics across species, including cell body size and distribution, the presence of a highly invaginated nucleus, and a well-developed system of cisternae. Reaction product was localized along the membranes of rough and smooth endoplasmic reticulum, subsurface cisternae, and the nuclear envelope. This label was distributed throughout the cartwheel cell body and dendritic shafts but not within dendritic spines, axons, or axon terminals. The regular pattern of immunolabeling across mammals suggests that IP3 and cartwheel cells are conserved in evolution and that both play an important but as yet unknown role in hearing.

IT 88269-39-0, Inositol 1,4,5-trisphosphate
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(receptors; immunocytochem. localization of inositol trisphosphate receptors in dorsal cochlear nucleus of mammals)
RN 88269-39-0 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Relative stereochemistry.



L7 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:265528 CAPLUS
DOCUMENT NUMBER: 122:47127
TITLE: Autoradiographic distribution of neurotransmitter and second messenger system receptors in animal brains
AUTHOR(S): Kanai, Yasuo; Araki, Tsutomu; Kato, Hiroyuki; Kogure, Kyuya

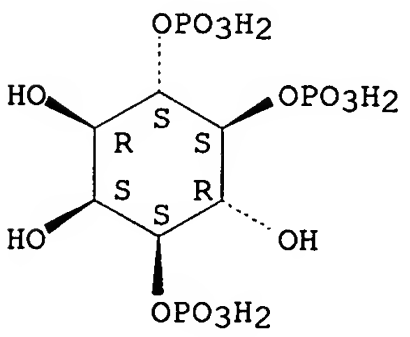
CORPORATE SOURCE: Pharmacological Research Laboratory, Tokyo Tanabe Co., Ltd., Kitami, 115, Japan
SOURCE: Behavioural Brain Research (1994), 65(1), 67-73
CODEN: BBREDI; ISSN: 0166-4328
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors investigated species difference in binding of major neurotransmitters and intracellular second messengers in the gerbil brain and the rat brain using receptor autoradiog. [3H]Phorbol 12,13-dibutyrate (PDBu), [3H]inositol 1,4,5-trisphosphate (IP3), [3H]PN200-110, [3H]muscimol, [3H]MK-801, [3H]cyclohexyladenosine (CHA), and [3H]quinuclidinyl benzilate (QNB) were used to label protein kinase C, IP3 receptor, L-type calcium channel, γ-aminobutyric acidA (GABAA) receptor, N-methyl-D-aspartate (NMDA) receptor, adenosine A1 receptor, and muscarinic cholinergic receptor, resp. Autoradiog. distributions of the bindings of most neurotransmitters and second messengers were particularly found in the limbic system and basal ganglia in both gerbil and rat brains. However, marked differences in these bindings between the gerbil brain and the rat brain were also recognized in the above regions. In particular, among 7 ligands used, the gerbil had high [3H]PDBu and [3H]CHA binding sites throughout the brain compared to those in the rat brain except for a few areas. By contrast, the rat exhibited high [3H]MK-801 binding sites in various brain regions, as compared with the gerbil brain. Thus, the gerbil differ from the rat with respect to the binding sites of major second messengers and neurotransmitters in the brain. The results may help better elucidate the relation or species difference between gerbils and rats for neuronal function and behavioral pharmacol.

IT 88269-39-0, Inositol 1,4,5 trisphosphate
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(species variation in neurotransmitter and second messenger system receptors in brains)

RN 88269-39-0 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Relative stereochemistry.



L7 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:221631 CAPLUS
DOCUMENT NUMBER: 122:102369
TITLE: Age-dependent changes in second messenger and rolipram receptor systems in the gerbil brain
AUTHOR(S): Araki, T.; Kato, H.; Kanai, Y.; Kogure, K.
CORPORATE SOURCE: Institute Brain Diseases, Tohoku University School Medicine, Sendai, Japan
SOURCE: Journal of Neural Transmission: General Section (1994), 97(2), 135-47
CODEN: JNGSE8; ISSN: 0300-9564
DOCUMENT TYPE: Journal
LANGUAGE: English

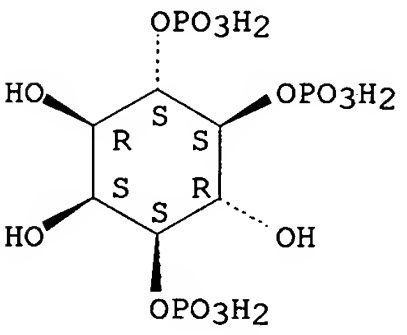
AB Age-related alterations in binding sites of major second messengers and a selective cAMP phosphodiesterase (PDE) in the gerbil brain were analyzed by receptor autoradiog. [3H]Phorbol 12,13-dibutyrate (PDBu), [3H]inositol 1,4,5-trisphosphate (IP3), [3H]forskolin, [3H]cAMP, and [3H]rolipram were used to label protein kinase C (PKC), IP3 receptor, adenylate cyclase, cAMP dependent protein kinase (PKA), and Ca2+/calmodulin-independent cAMP PDE, resp. In middle-aged gerbils (16 mo old), [3H]PDBu binding was significantly reduced in the hippocampal CA1 sector, thalamus, substantia nigra, and cerebellum, compared with young animals (1 mo old). [3H]IP3 binding revealed significant elevations in the nucleus accumbens, hippocampal CA1 sector, dentate gyrus, and a significant reduction in cerebellum of middle-aged gerbils. [3H]Forskolin binding in middle-aged animals was significantly increased in the nucleus accumbens and hilus of dentate gyrus, but was diminished in the substantia nigra and cerebellum. In middle-aged animals, [3H]cAMP binding revealed a significant elevation only in the hippocampal CA3 sector, whereas [3H]rolipram binding showed a significant reduction in the thalamus and cerebellum. Thus, the age-related alteration in these binding sites showed different patterns among various brain regions in middle-aged gerbils indicating that the binding sites of PKC, IP3, and adenylate cyclase are more markedly affected by aging than those of PKA and cAMP PDE and that the hippocampus and cerebellum are more susceptible to these aging processes than other brain regions. The findings suggest that intracellular signal transduction is affected at an early stage of senescence and this may lead to neurol. deficits.

IT 88269-39-0, Inositol 1,4,5-trisphosphate
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(second messenger and calcium-calmodulin-independent cAMP phosphodiesterase receptors of brain in senescence)

RN 88269-39-0 CAPLUS

CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Relative stereochemistry.



L7 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1993:249997 CAPLUS

DOCUMENT NUMBER: 118:249997

TITLE: Inositol 1,4,5-trisphosphate receptors: Labeling the inositol 1,4,5-trisphosphate binding site with photoaffinity ligands

AUTHOR(S): Mourey, Robert J.; Estevez, Virginia A.; Marecek, James F.; Barrow, Roxanne K.; Prestwich, Glenn D.; Snyder, Solomon H.

CORPORATE SOURCE: Dep. Neurosci., Johns Hopkins Med. Inst., Baltimore, MD, 21205, USA

SOURCE: Biochemistry (1993), 32(7), 1719-26
CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE: Journal

LANGUAGE: English

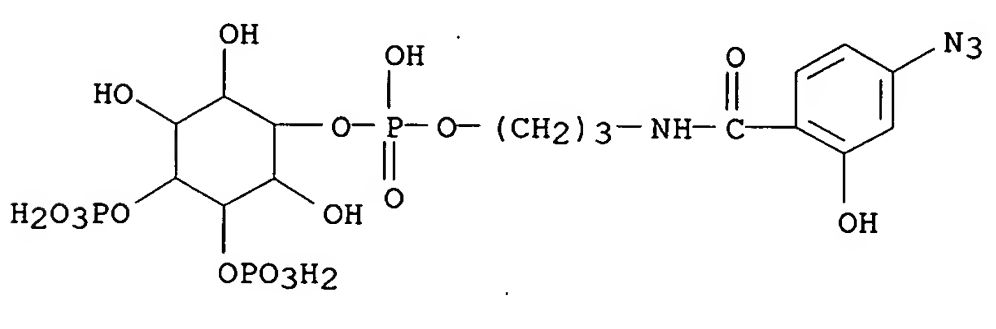
AB The inositol 1,4,5-trisphosphate (IP3) receptor was

photolabeled and the IP3 ligand binding site was probed using two novel photoaffinity ligands, [125I](azidosalicyl)aminopropyl-IP3 ([125I]ASA-IP3) and [3H](benzoyldihydrocinnamyl)aminopropyl-IP3 ([3H]BZDC-IP3). Both ligands have high affinity for the IP3 receptor and, when photoactivated, label the IP3 receptor protein with appropriate inositol phosphate selectivity. The high specific activity of [125I]ASA-IP3 allowed identification of a single photolabeling site within the IP3R by two-dimensional peptide anal. Substantially higher levels of incorporation into the receptor are achieved with [3H]BZDC-IP3 (50-60% efficiency) than with [125I]ASA-IP3 (3%), facilitating the use of [3H]BZDC-IP3 as a better ligand for the high-efficiency labeling and purification of IP3R-labeled peptides. Peptides were generated from photolabeled IP3 receptor by trypsin digestion and purified by high-pressure liquid chromatog. (HPLC). A single purified [3H]BZDC-IP3-labeled peptide, corresponding to IP3R amino acids 476-501, was sequenced and shown to match specific sequences in the N-terminal 20% of the IP3 receptor, an area suggested on the basis of mutagenesis studies to contain the IP3 recognition site.

IT 147852-81-1
RL: BIOL (Biological study)
(inositol trisphosphate receptor photoaffinity labeling with)

RN 147852-81-1 CAPLUS

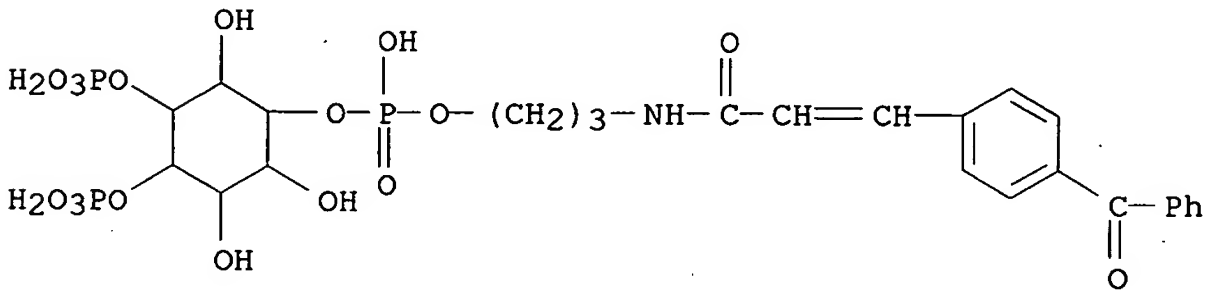
CN myo-Inositol, 1-[3-[(4-azido-2-hydroxybenzoyl)amino]propyl hydrogen phosphate] 4,5-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)



IT 147764-82-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation or tritiation of)

RN 147764-82-7 CAPLUS

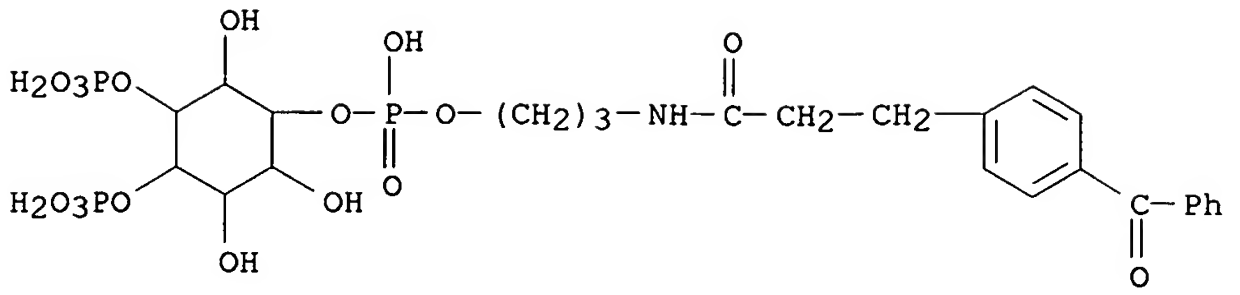
CN myo-Inositol, 1-[3-[[3-(4-benzoylphenyl)-1-oxo-2-propenyl]amino]propyl hydrogen phosphate] 4,5-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)



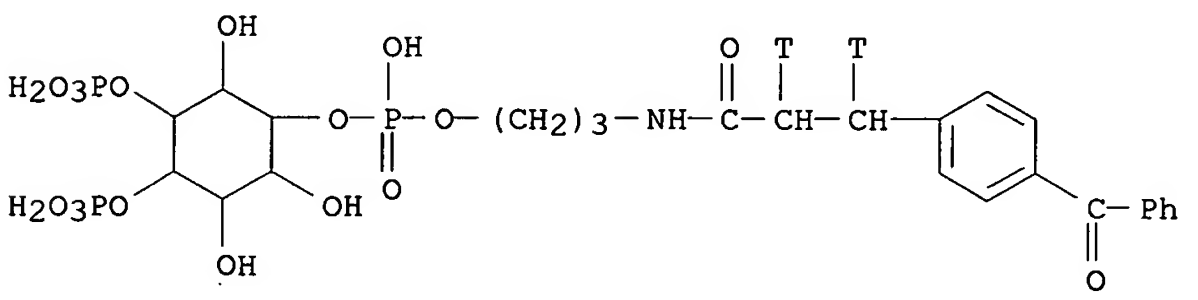
IT 147764-83-8P 147764-84-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and inositol trisphosphate receptor photoaffinity labeling with)

RN 147764-83-8 CAPLUS

CN myo-Inositol, 1-[3-[[3-(4-benzoylphenyl)-1-oxopropyl]amino]propyl hydrogen phosphate] 4,5-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

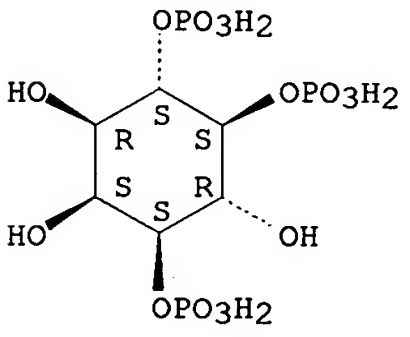


RN 147764-84-9 CAPLUS
CN myo-Inositol, 1-[3-[[3-(4-benzoylphenyl)-1-oxopropyl-2,3-t2]amino]propyl hydrogen phosphate] 4,5-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)



IT 88269-39-0, Inositol 1,4,5-trisphosphate
RL: BIOL (Biological study)
(receptor of cerebellum membrane binding site for, identification of, by photoaffinity labeling)
RN 88269-39-0 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Relative stereochemistry.



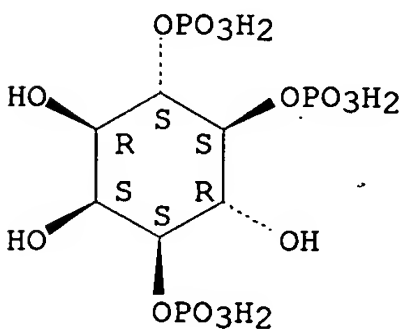
L7 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:529224 CAPLUS
DOCUMENT NUMBER: 117:129224
TITLE: Mapping of second messenger and rolipram receptors in mammalian brain
AUTHOR(S): Araki, Tsutomu; Kato, Hiroyuki; Kogure, Kyuya
CORPORATE SOURCE: Sch. Med., Tohoku Univ., Sendai, Japan
SOURCE: Brain Research Bulletin (1992), 28(6), 843-8
CODEN: BRBUDU; ISSN: 0361-9230
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Autoradiog. localization of major second messengers and cAMP phosphodiesterase in the brain were visualized in the gerbil and rat using receptor autoradiog. [3H]phorbol 12,13-dibutyrate (PDBu), [3H]inositol 1,4,5-trisphosphate (IP3), [3H]forskolin, [3H]cAMP, and [3H]rolipram were

used to label protein kinase C, IP3 receptors , adenylate cyclase, cAMP-dependent protein kinase (cAMP-DPK), and Ca2+/calmodulin-independent cAMP phosphodiesterase (PDE), resp. Most second messengers and rolipram binding activities were found in the limbic system, basal ganglia, and cerebellum. Marked differences were noted in the hippocampus, where cAMP and rolipram binding activities were very low in gerbils but high in rats. The regional localization in the binding sites of PDBu, IP3, and forskolin in the gerbil and rat brains was similar. Alteration of the cAMP and rolipram binding sites was studied in the gerbil hippocampus 7 days after a 10-min cerebral ischemia. The results suggest that the gerbil differs from the rat with respect to the characteristic neurons or interneurons, especially in the hippocampal formation.

This finding may elucidate the relationship or difference between gerbils and rats in brain functions and behavioral pharmacol. The cAMP and rolipram binding sites may be predominantly distributed on the pyramidal cell layer of the hippocampal CA1 sector and transient cerebral ischemia can cause marked reduction of these binding sites in the hippocampus.

IT 88269-39-0, Inositol 1,4,5-trisphosphate
RL: BIOL (Biological study)
(brain receptors for, ischemia and species in relation to)
RN 88269-39-0 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Relative stereochemistry.



L7 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:490704 CAPLUS
DOCUMENT NUMBER: 117:90704
TITLE: Preparation of inositol polyphosphate derivatives for control of the calcium ion-participating metabolic steps
INVENTOR(S): Ozaki, Shoichiro; Watanabe, Yutaka; Hirata, Masato; Awaya, Akira
PATENT ASSIGNEE(S): Mitsui Toatsu Chemicals, Inc., Japan
SOURCE: PCT Int. Appl., 139 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

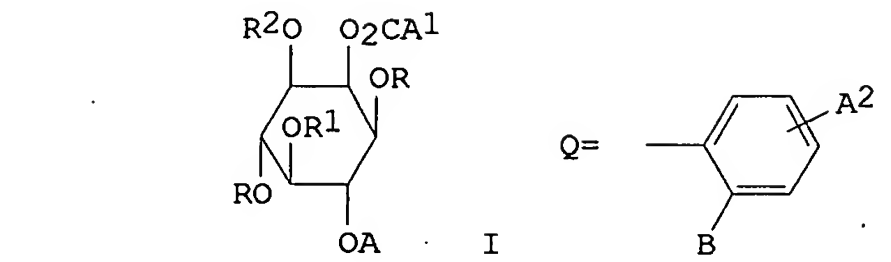
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9104258	A1	19910404	WO 1990-JP1228	19900925
W: US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE				
EP 445299	A1	19910911	EP 1990-913864	19900925
R: CH, DE, FR, GB, IT, LI				
JP 04178394	A	19920625	JP 1990-251804	19900925
US 5252707	A	19931012	US 1991-700152	19910515

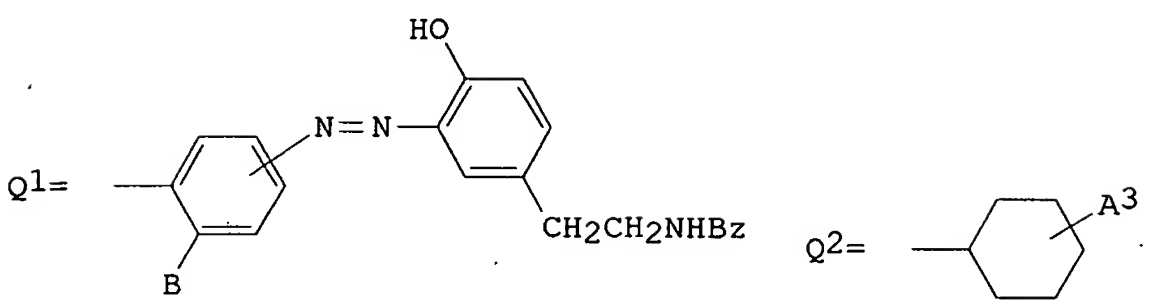
PRIORITY APPLN. INFO.:

JP 1989-245161	A	19890922
JP 1990-210263	A	19900810
WO 1990-JP1228	W	19900925

OTHER SOURCE(S): MARPAT 117:90704

GI



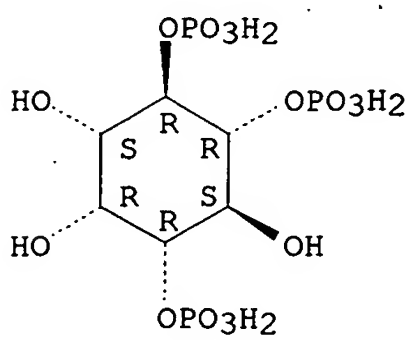


AB The title compds. [I; A = H; R,R1 = (un)protected P(O)(OH)2 and R2 = H; R,R2 = (un)protected P(O)(OH)2, R1 = H; or R,R1,R2 = (un)protected P(O)(OH)2; A1 = (CH2)nCHR3NH2, Q, Q1, Q2, (CH2)nCHR3N:CR4N5, (CH2)nCHR3NHCO2R6, etc.; n = 0-5; R3 = H, (hydroxy)alkyl; (p-hydroxy)phenyl, (p-hydroxy)benzyl, 3-methylindolyl, 5-methylimidazolyl, etc.; R4, R5, R6 = H, alkyl, alkenyl, alkynyl, (un)substituted Ph or cyclohexyl; A2, A3 = N3, NH2, N:CR4R5, NHCHR4R5, etc.; B = H, NH2, NHCOCF3] which are used as drugs having 1,3,4-IP3-, IP3-, or IP4- (IP3, IP4 = inositol tri-orthotetraphosphate, resp.) like activities or antagonizing the activities of 1,3,4-IP3, IP3, or IP4 formed in vivo, and conjugates of I with polypeptides or proteins which are used as diagnostic agents and health foods, are prepared I immobilized on a solid support are also prepared and can be used for separation and purification of IP3 phosphatase, IP4 phosphatase, IP3 kinase, IP4 kinase, IP3 receptor and IP4 receptor. Addnl. prepared are I linked to biotin or a fluorescent substance useful as biotin-avidin complex probes of fluorescent probes for studying the structure-activity relationship, the mechanism of action, or the search of the active site of proteins having affinity towards inositol phosphate-related phosphatase, kinase, and receptors. Thus, hydrogenation of I [A = R2 = CH2Ph, R = R1 = P(O)(OCH2Ph)2, A1 = p-(O2N)C6H4CO] over 5% Pd/C in aqueous MeOH containing AcONH4 gave 100% I [A = R2 = H, R = R1 = P(O)(OH)2, A1 = p-(H2N)C6H4CO] as the NH3 salt (II) which was hydrogenated over RuO2 in H2O at 80 atm H and 60° to give I [A = R2 = H, R = R1 = P(O)(OH)2, A1 = 4-aminocyclohexanecarbonyl] as the NH3 salt (III). II and III in vitro showed IC50 of 3 and 4.2 nM for inhibiting the binding of [3H]IP3 to the microsome of bovine adrenal cortex, resp. vs. 1.4 nM for IP3 and EC50 of 1.6 and 1.2 μM, resp. for releasing Ca2+ from microphages of guinea pigs abdominal cavity vs. 0.2 μM for IP3.

IT 85166-31-0, Inositol triphosphate 98102-63-7, 1,3,4-Inositol triphosphate
RL: RCT (Reactant); RACT (Reactant or reagent)
(agonists or antagonists, inositol tri- or tetraphosphate derivs.)

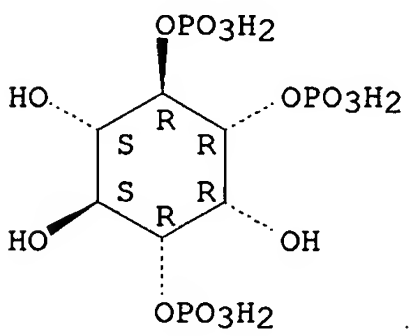
RN 85166-31-0 CAPLUS
CN D-myo-Inositol, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

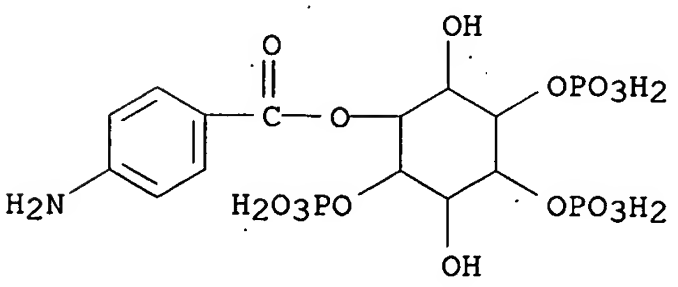


RN 98102-63-7 CAPLUS
CN myo-Inositol, 1,3,4-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

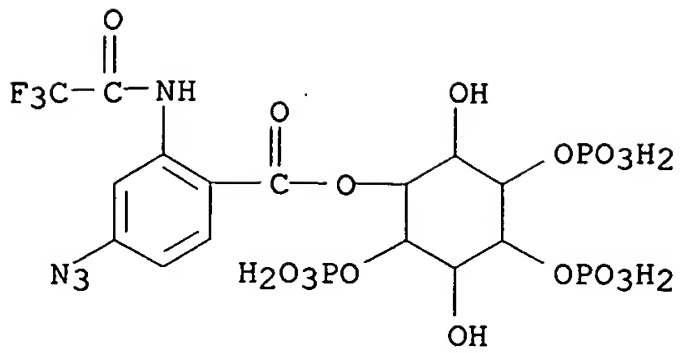
Relative stereochemistry.



IT 128443-67-4P 135417-68-4P 135417-70-8P
135417-71-9P 135417-72-0P 135417-73-1P
135417-74-2P 135417-75-3P 135417-76-4P
135417-77-5P 135417-78-6P 135417-79-7P
135417-80-0P 135417-81-1P 135417-82-2P
135442-09-0P 135502-62-4P 135502-63-5P
135502-64-6P 135502-65-7P 135502-66-8P
135502-67-9P 135502-68-0P 135502-69-1P
135502-70-4P 135502-71-5P 135502-72-6P
135502-73-7P 135556-66-0P 135556-67-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn of, for regulation of calcium ion-mediated metabolism)
RN 128443-67-4 CAPLUS
CN D-myo-Inositol, 2-(4-aminobenzoate) 1,4,5-tris(dihydrogen phosphate) (9CI)
(CA INDEX NAME)



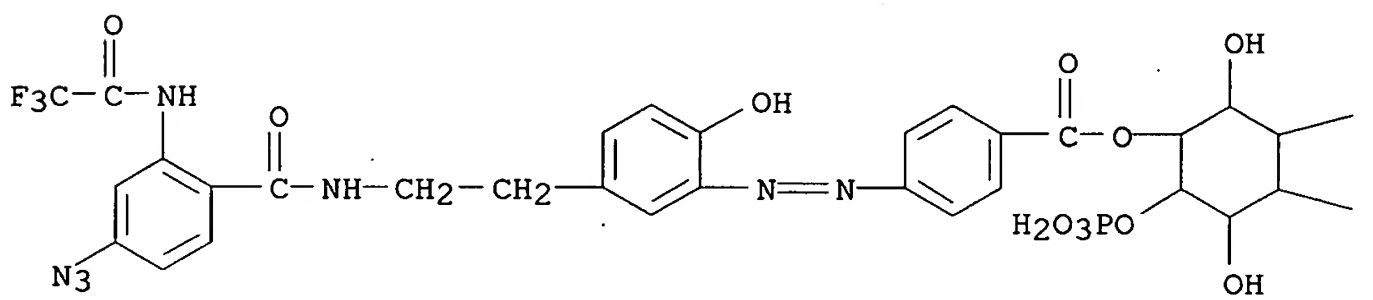
RN 135417-68-4 CAPLUS
CN myo-Inositol, 2-[4-azido-2-[(trifluoroacetyl)amino]benzoate]
1,4,5-tris(dihydrogen phosphate), monoammonium salt (9CI) (CA INDEX NAME)



● NH_3

RN 135417-70-8 CAPLUS
CN myo-Inositol, 2-[4-[[5-[2-[[4-azido-2-[(trifluoroacetyl)amino]benzoyl]amino]ethyl]-2-hydroxyphenyl]azo]benzoate] 1,4,5-tris(dihydrogen phosphate), monoammonium salt (9CI) (CA INDEX NAME)

PAGE 1-A



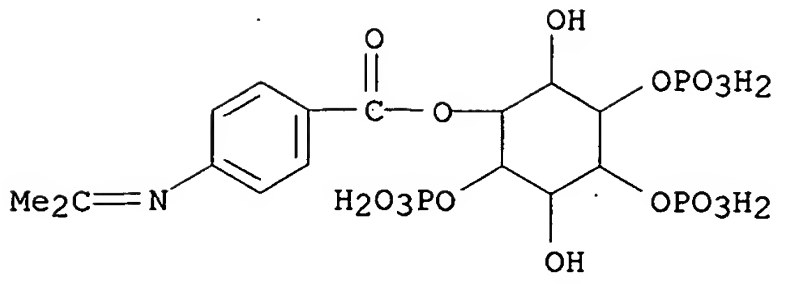
● NH_3

PAGE 1-B

OPO_3H_2

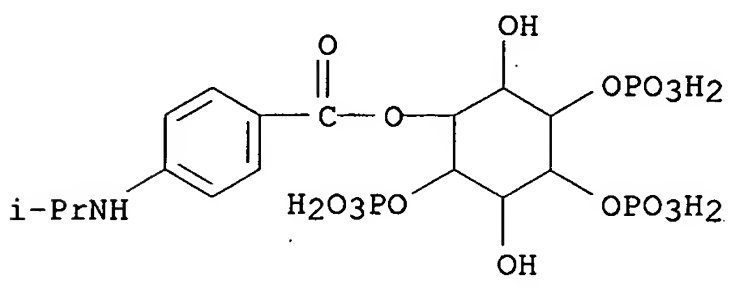
OPO_3H_2

RN 135417-71-9 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) 2-[4-[(1-methylethylidene)amino]benzoate], monopotassium salt (9CI) (CA INDEX NAME)



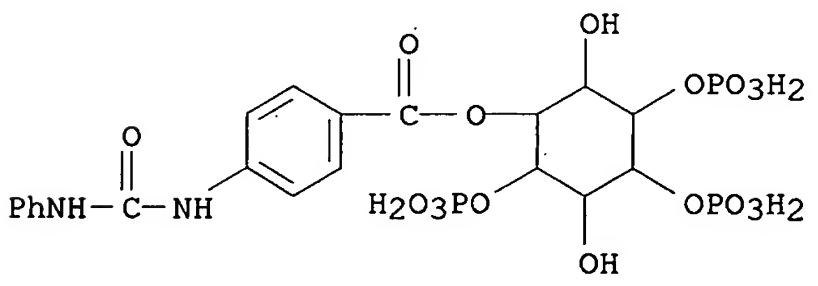
● K

RN 135417-72-0 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) 2-[4-[(1-methylethyl)amino]benzoate], monopotassium salt (9CI) (CA INDEX NAME)



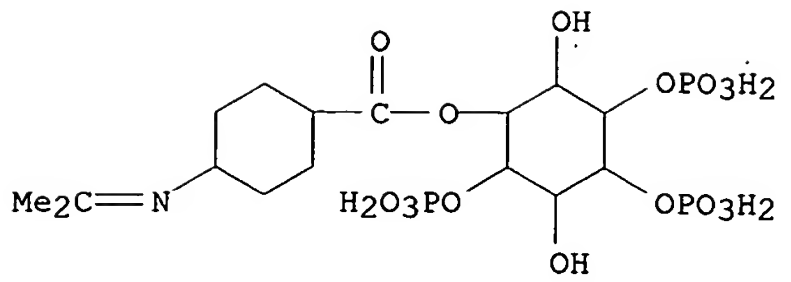
● K

RN 135417-73-1 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) 2-[4-[[(phenylamino)carbonyl]amino]benzoate], monopotassium salt (9CI) (CA INDEX NAME)



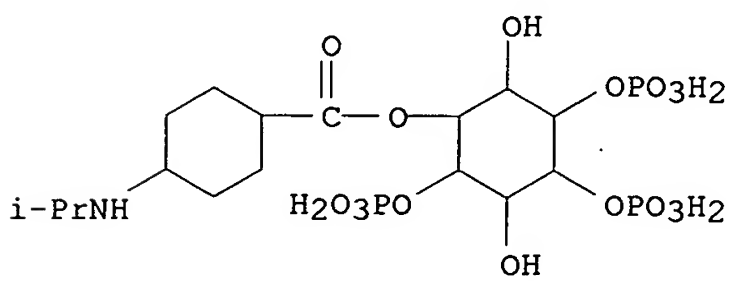
● K

RN 135417-74-2 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) 2-[4-[(1-methylethylidene)amino]cyclohexanecarboxylate], monopotassium salt (9CI) (CA INDEX NAME)



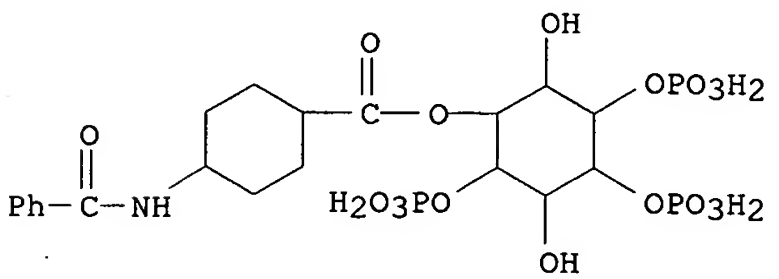
● K

RN 135417-75-3 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) 2-[4-[(1-methylethyl)amino]cyclohexanecarboxylate], monopotassium salt (9CI) (CA INDEX NAME)



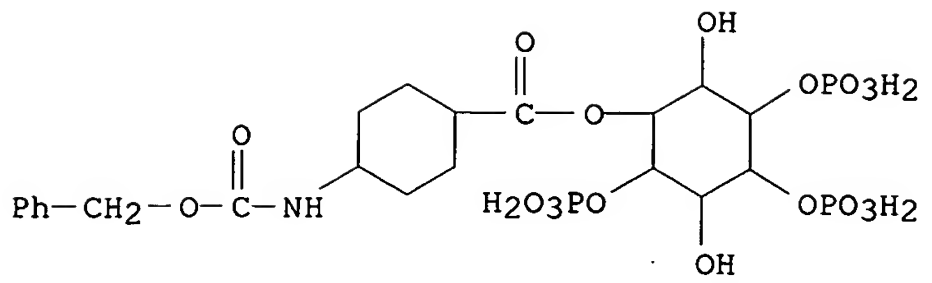
● K

RN 135417-76-4 CAPLUS
CN myo-Inositol, 2-[4-(benzoylamino)cyclohexanecarboxylate] 1,4,5-tris(dihydrogen phosphate), tripotassium salt (9CI) (CA INDEX NAME)



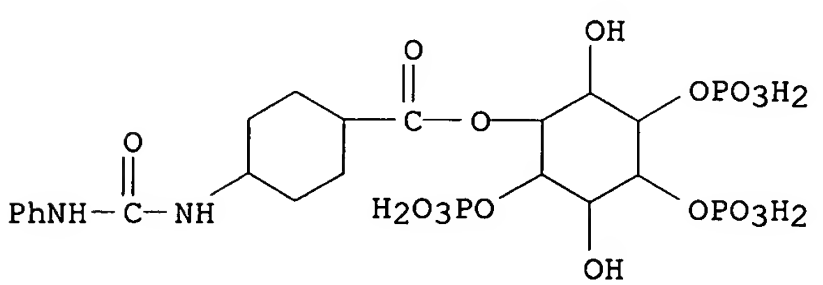
●3 K

RN 135417-77-5 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) 2-[4-[[(phenylmethoxy)carbonyl]amino]cyclohexanecarboxylate], tripotassium salt (9CI) (CA INDEX NAME)



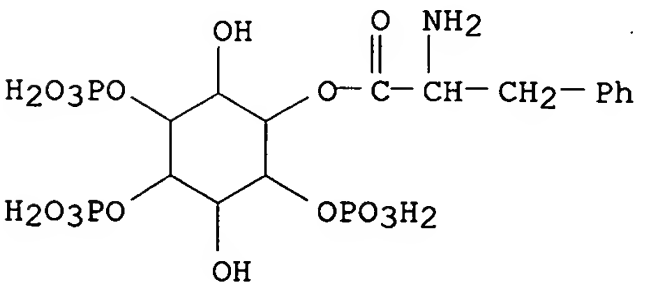
●3 K

RN 135417-78-6 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) 2-[4-[[(phenylamino)carbonyl]amino]cyclohexanecarboxylate], tripotassium salt (9CI) (CA INDEX NAME)



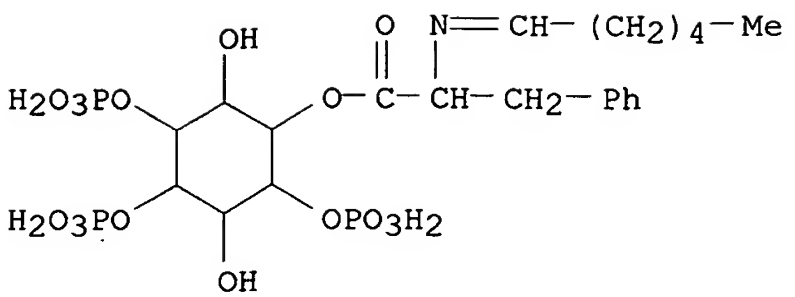
●3 K

RN 135417-79-7 CAPLUS
CN L-Phenylalanine, 2-ester with D-myo-inositol 1,4,5-tris(dihydrogen phosphate), triammonium salt (9CI) (CA INDEX NAME)



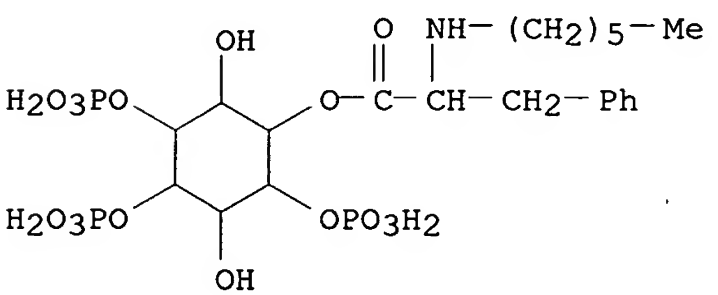
●3 NH_3

RN 135417-80-0 CAPLUS
CN L-Phenylalanine, N-hexylidene-, 2-ester with myo-inositol 1,4,5-tris(dihydrogen phosphate), monopotassium salt (9CI) (CA INDEX NAME)



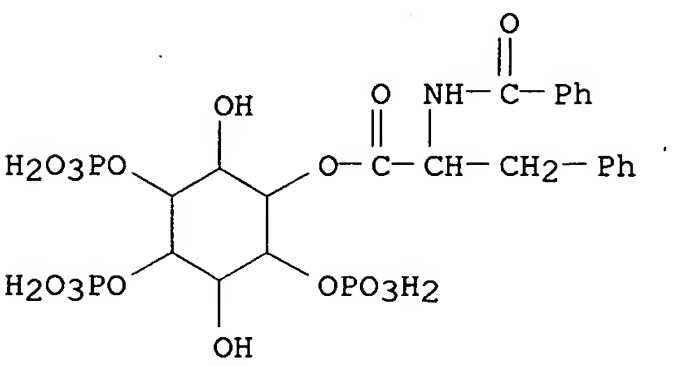
● K

RN 135417-81-1 CAPLUS
CN L-Phenylalanine, N-hexyl-, 2-ester with myo-inositol 1,4,5-tris(dihydrogen phosphate), monopotassium salt (9CI) (CA INDEX NAME)



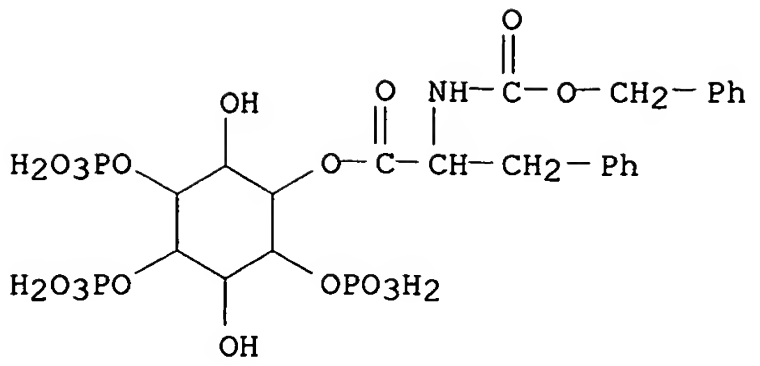
● K

RN 135417-82-2 CAPLUS
CN L-Phenylalanine, N-benzoyl-, 2-ester with myo-inositol 1,4,5-tris(dihydrogen phosphate), tripotassium salt (9CI) (CA INDEX NAME)



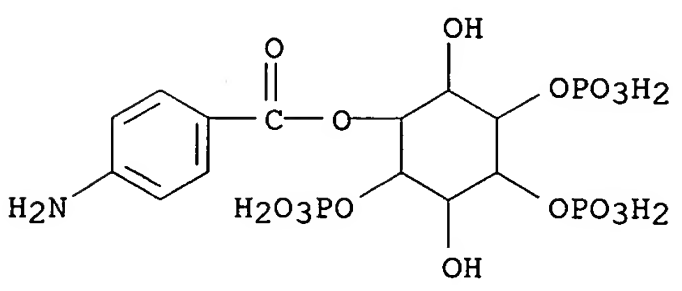
●3 K

RN 135442-09-0 CAPLUS
CN L-Phenylalanine, N-[(phenylmethoxy)carbonyl]-, 2-ester with myo-inositol 1,4,5-tris(dihydrogen phosphate), tripotassium salt (9CI) (CA INDEX NAME)



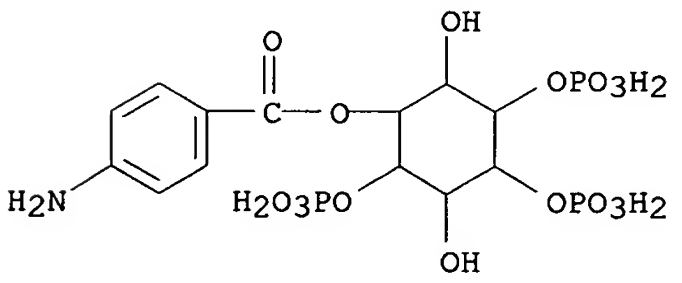
● 3 K

RN 135502-62-4 CAPLUS
CN D-myo-Inositol, 2-(4-aminobenzoate) 1,4,5-tris(dihydrogen phosphate), monoammonium salt (9CI) (CA INDEX NAME)



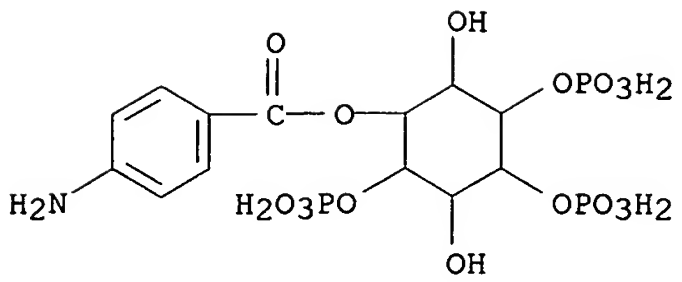
● NH_3

RN 135502-63-5 CAPLUS
CN D-myo-Inositol, 2-(4-aminobenzoate) 3,5,6-tris(dihydrogen phosphate), monoammonium salt (9CI) (CA INDEX NAME)



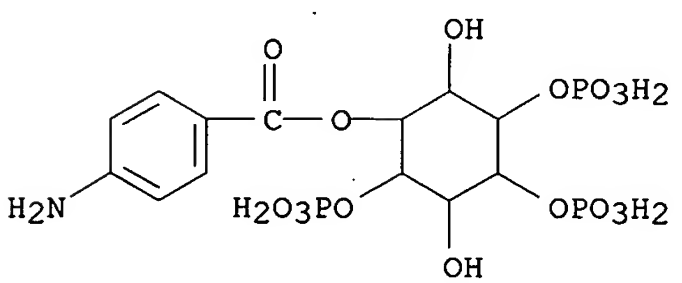
● NH_3

RN 135502-64-6 CAPLUS
CN D-myo-Inositol, 2-(4-aminobenzoate) 1,4,5-tris(hydrogen phosphate), trisodium salt (9CI) (CA INDEX NAME)



●3 Na

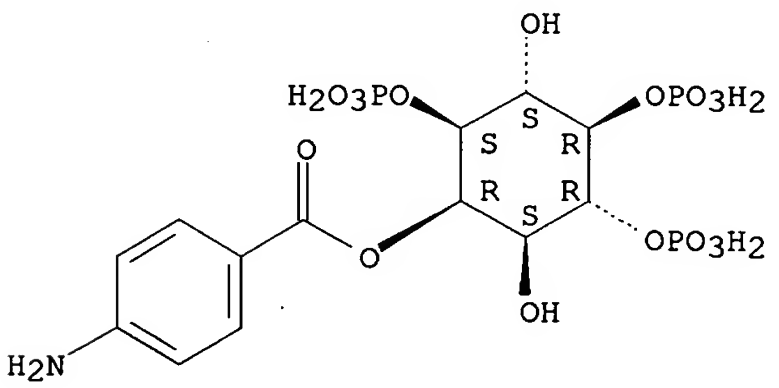
RN 135502-65-7 CAPLUS
CN D-myo-Inositol, 2-(4-aminobenzoate) 3,5,6-tris(dihydrogen phosphate), trisodium salt (9CI) (CA INDEX NAME)



●3 Na

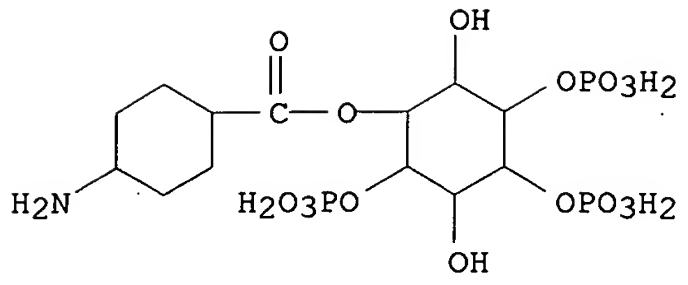
RN 135502-66-8 CAPLUS
CN myo-Inositol, 2-(4-aminobenzoate) 1,4,5-tris(dihydrogen phosphate), monosodium salt (9CI) (CA INDEX NAME)

Relative stereochemistry.



● Na

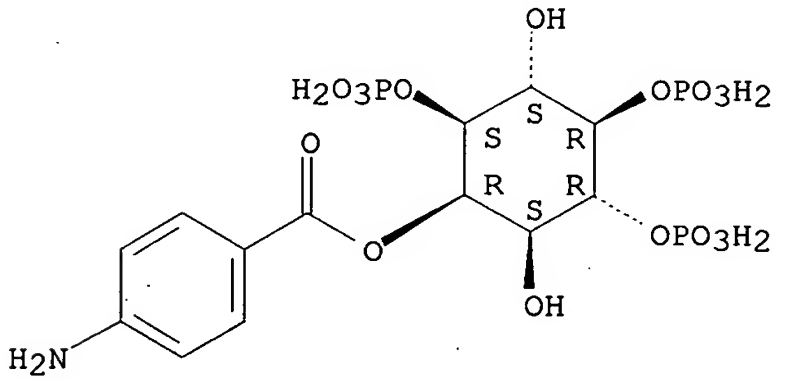
RN 135502-67-9 CAPLUS
CN myo-Inositol, 2-(4-aminocyclohexanecarboxylate) 1,4,5-tris(dihydrogen phosphate), monosodium salt (9CI) (CA INDEX NAME)



● Na

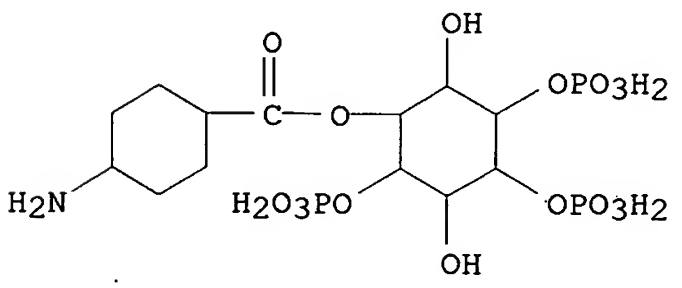
RN 135502-68-0 CAPLUS
CN myo-Inositol, 2-(4-aminobenzoate) 1,4,5-tris(dihydrogen phosphate), monoammonium salt (9CI) (CA INDEX NAME)

Relative stereochemistry.



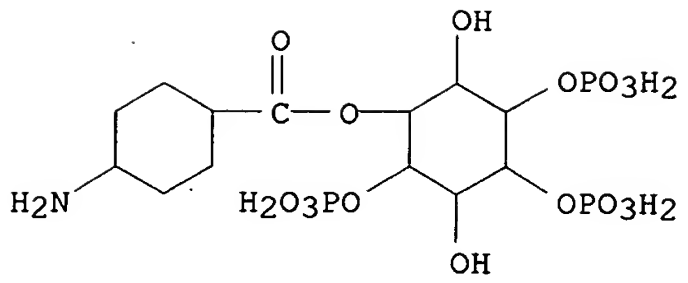
● NH_3

RN 135502-69-1 CAPLUS
CN D-myo-Inositol, 2-(4-aminocyclohexanecarboxylate) 1,4,5-tris(dihydrogen phosphate), monoammonium salt (9CI) (CA INDEX NAME)



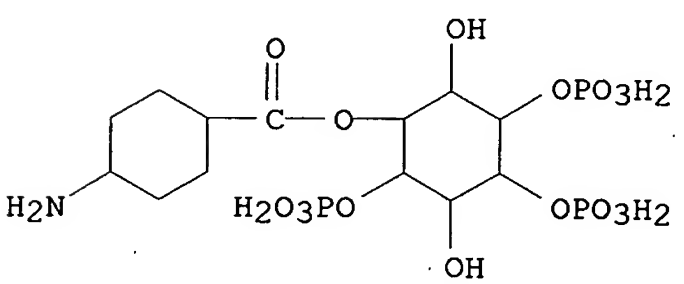
● NH_3

RN 135502-70-4 CAPLUS
CN D-myo-Inositol, 2-(4-aminocyclohexanecarboxylate) 3,5,6-tris(dihydrogen phosphate), monoammonium salt (9CI) (CA INDEX NAME)



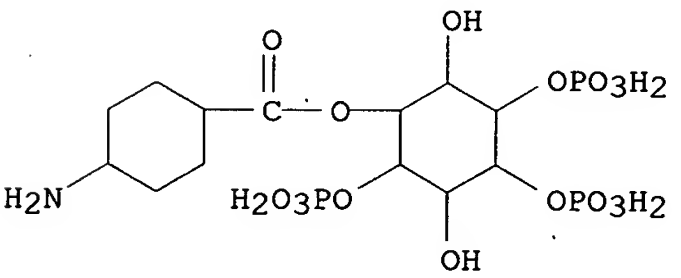
● NH_3

RN 135502-71-5 CAPLUS
CN D-myo-Inositol, 2-(4-aminocyclohexanecarboxylate) 1,4,5-tris(dihydrogen phosphate), trisodium salt (9CI) (CA INDEX NAME)



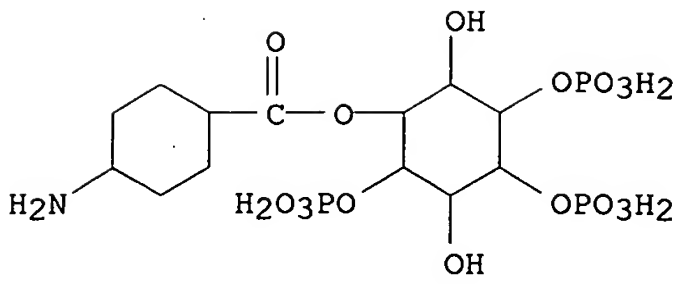
●3 Na

RN 135502-72-6 CAPLUS
CN D-myo-Inositol, 2-(4-aminocyclohexanecarboxylate) 3,5,6-tris(dihydrogen phosphate), trisodium salt (9CI) (CA INDEX NAME)



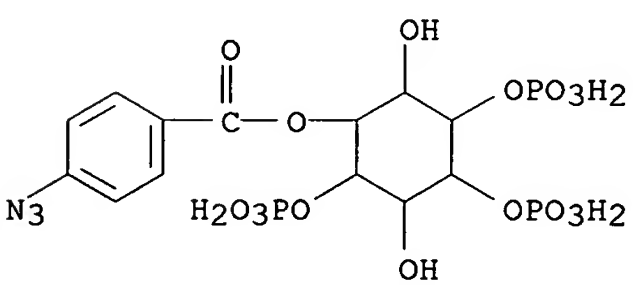
●3 Na

RN 135502-73-7 CAPLUS
CN myo-Inositol, 2-(4-aminocyclohexanecarboxylate) 1,4,5-tris(hydrogen phosphate), monoammonium salt (9CI) (CA INDEX NAME)



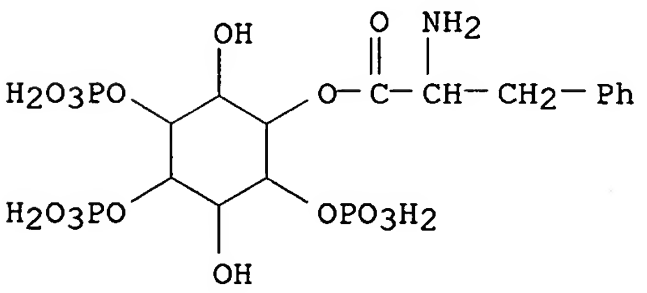
● NH_3

RN 135556-66-0 CAPLUS
CN myo-Inositol, 2-(4-azidobenzoate) 1,4,5-tris(dihydrogen phosphate), monoammonium salt (9CI) (CA INDEX NAME)



● NH_3

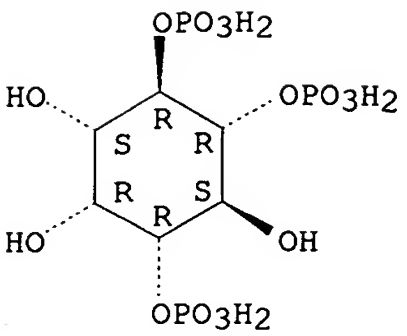
RN 135556-67-1 CAPLUS
CN L-Phenylalanine, 2-ester with D-myo-inositol 1,4,5-tris(dihydrogen phosphate), trisodium salt (9CI) (CA INDEX NAME)



●3 Na .

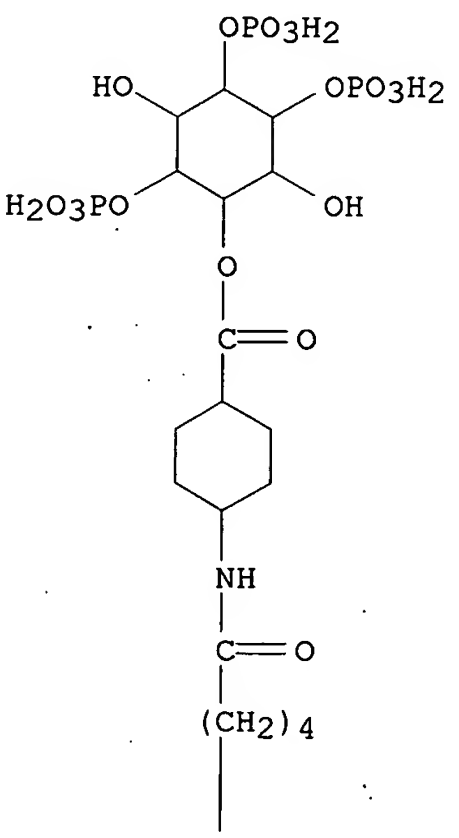
IT 85166-31-0DP, D-myo-Inositol 1,4,5-triphosphate, biotin-labeled
135417-83-3P 135417-84-4P 135417-85-5P
135442-10-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as biotin-avidin complex probe)
RN 85166-31-0 CAPLUS
CN D-myo-Inositol, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

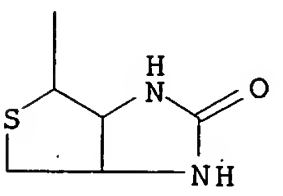


RN 135417-83-3 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) 2-[4-[[5-(hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl)-1-oxopentyl]amino]cyclohexanecarboxylate], monopotassium salt, [3aS-(3aα,4β,6aα)]- (9CI) (CA INDEX NAME)

PAGE 1-A



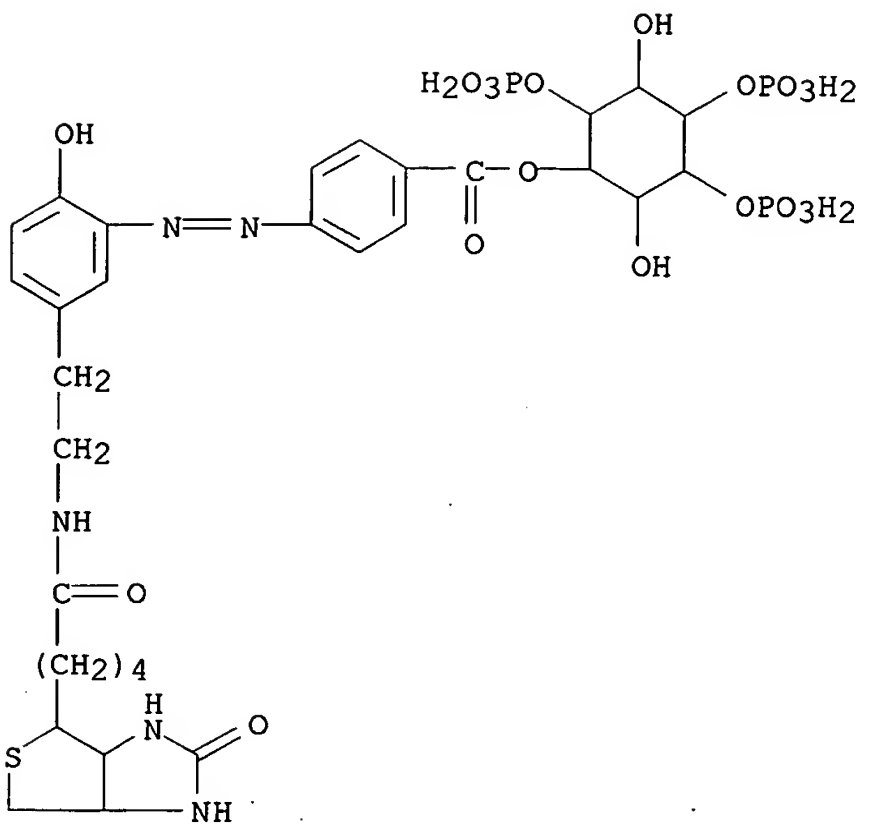
PAGE 2-A



● K

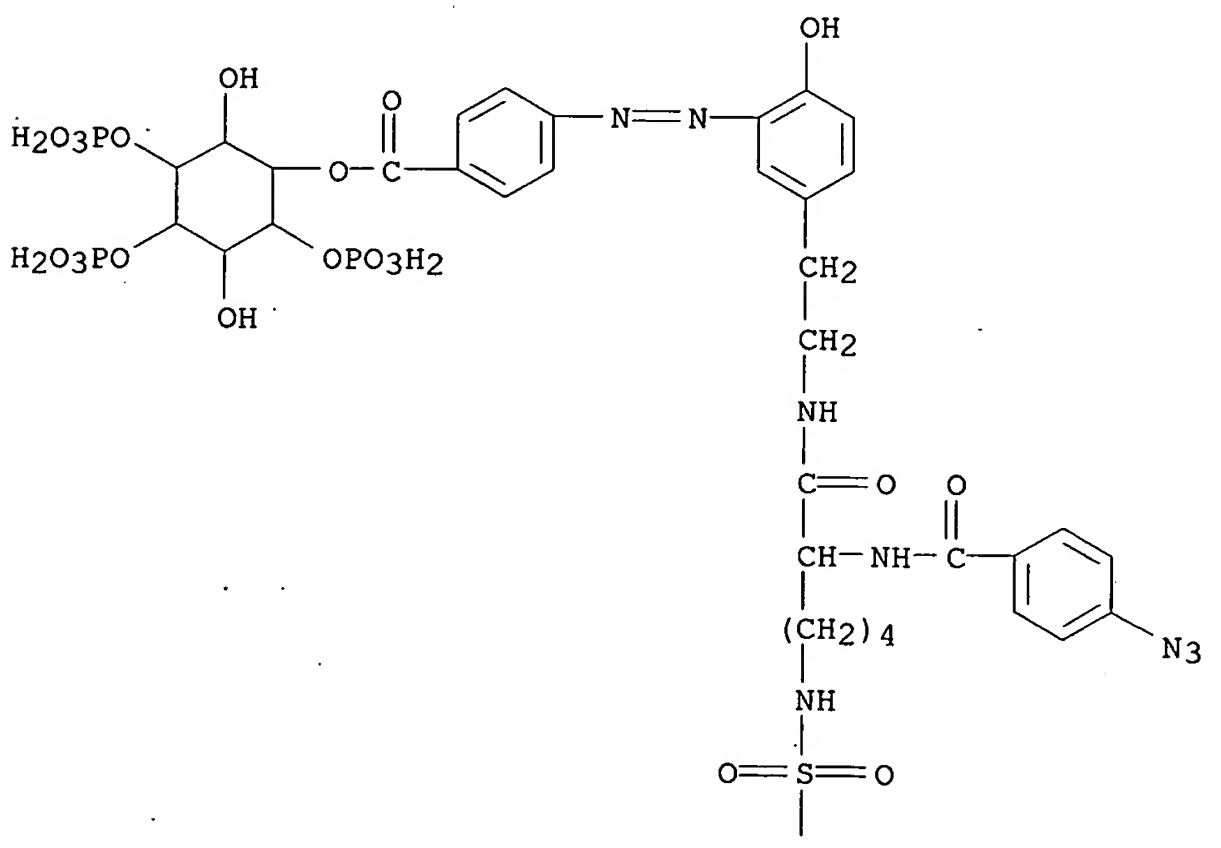
RN 135417-84-4 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) 2-[4-[[5-[2-[[5-(hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl)-1-oxopentyl]amino]ethyl]-2-hydroxyphenyl]azo]benzoate], monopotassium salt, [3aS-

(3aα,4β,6aα)]- (9CI) (CA INDEX NAME)

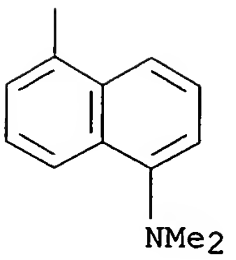


● K

RN 135417-85-5 CAPLUS
CN myo-Inositol, 2-[4-[[5-[2-[[2-[(4-azidobenzoyl)amino]-6-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]-1-oxohexyl]amino]ethyl]-2-hydroxyphenyl]azo]benzoate] 1,4,5-tris(dihydrogen phosphate), monopotassium salt, (S)- (9CI) (CA INDEX NAME)



PAGE 2-A

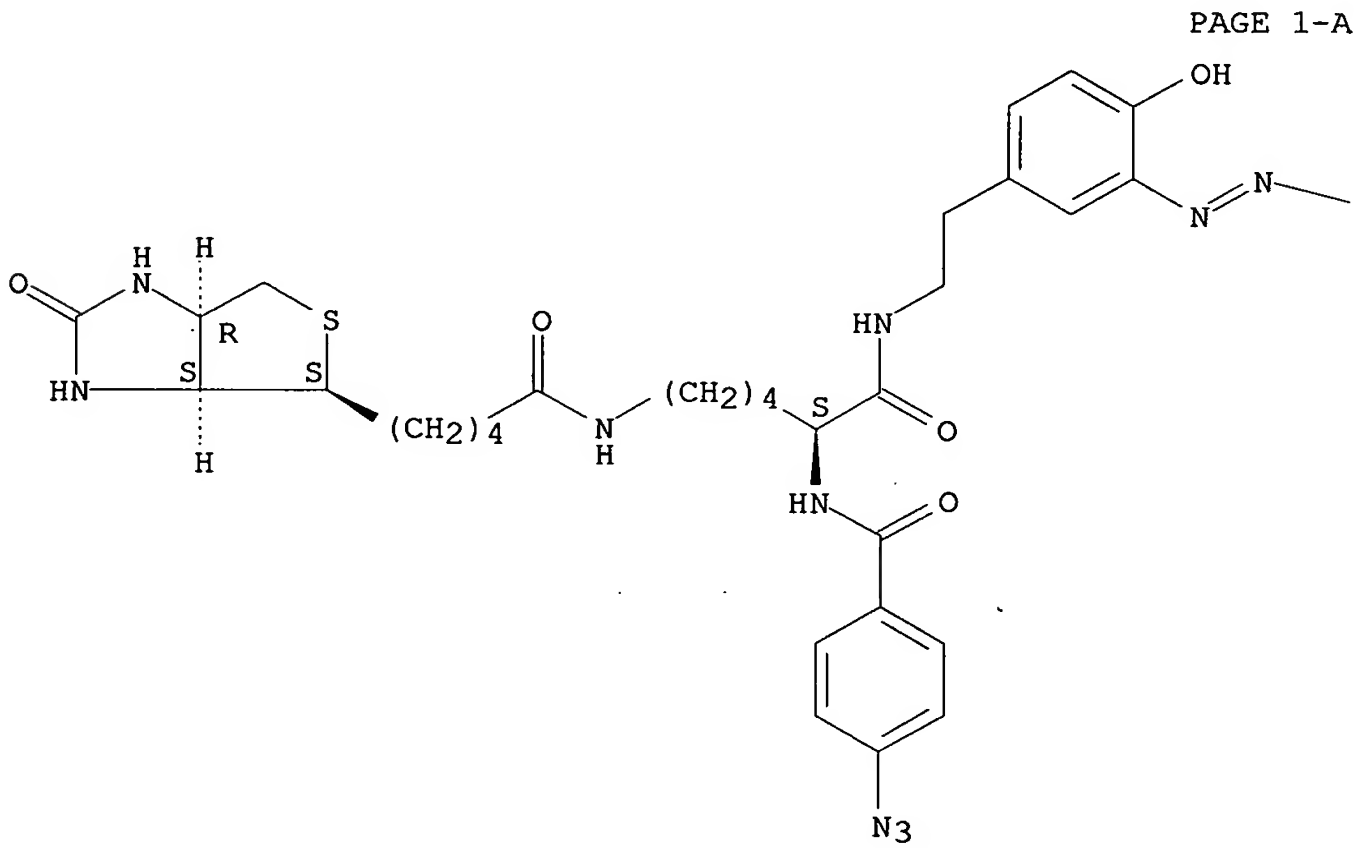


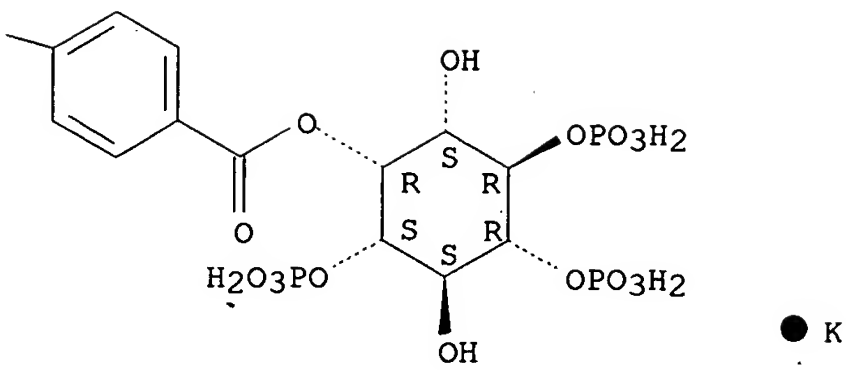
● K

RN 135442-10-3 CAPLUS
CN D-myo-Inositol, 2-[4-[[5-[2-[[(2S)-2-[(4-azidobenzoyl)amino]-6-[[5-[(3aS,4S,6aR)-hexahydro-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]amino]-1-oxohexyl]amino]ethyl]-2-hydroxyphenyl]azo]benzoate] 1,4,5-tris(dihydrogen phosphate), monopotassium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

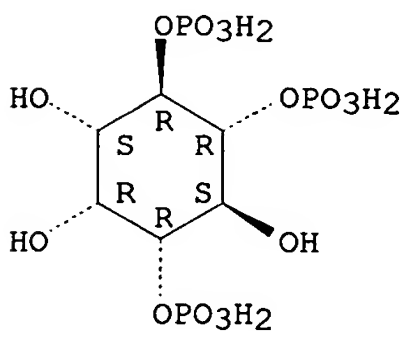
PAGE 1-A



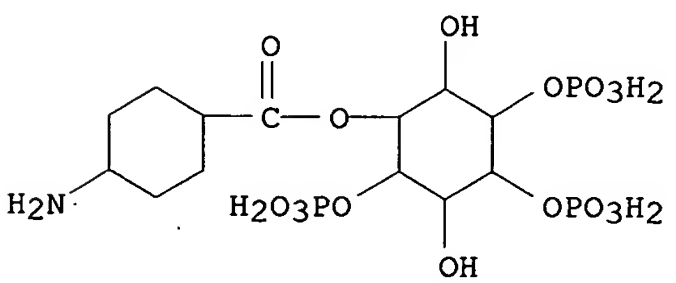


IT 85166-31-0DP, D-myo-Inositol 1,4,5-triphosphate, conjugates with proteins
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as diagnostic agents and health foods)
RN 85166-31-0 CAPLUS
CN D-myo-Inositol, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

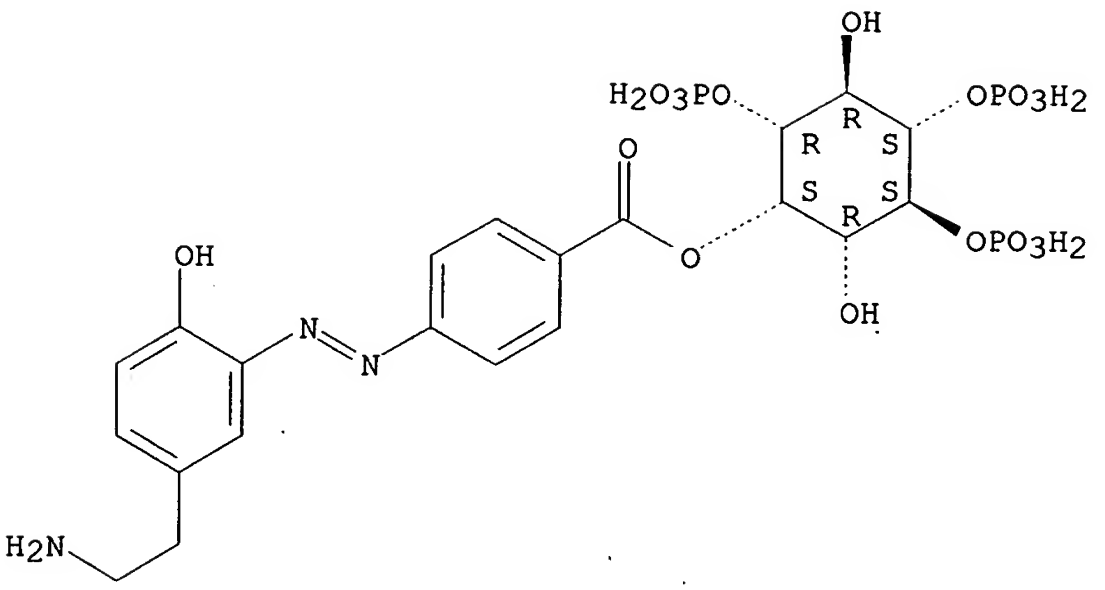


RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as fluorescent probe
IT 128443-66-3DP, CH-Sepharose 4B-bound 135502-74-8DP, CH-Sepharose 4B-bound
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for separation and purification of inositol tri- or tetraphosphate-phosphatase or kinase)
RN 128443-66-3 CAPLUS
CN D-myo-Inositol, 2-(4-aminocyclohexanecarboxylate) 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

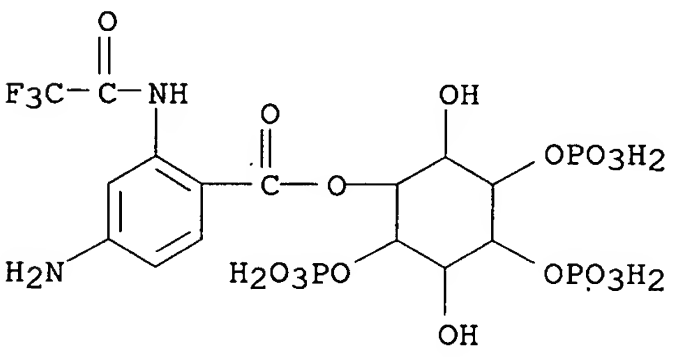


RN 135502-74-8 CAPLUS
CN myo-Inositol, 2-[4-[[5-(2-aminoethyl)-2-hydroxyphenyl]azo]benzoate] 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



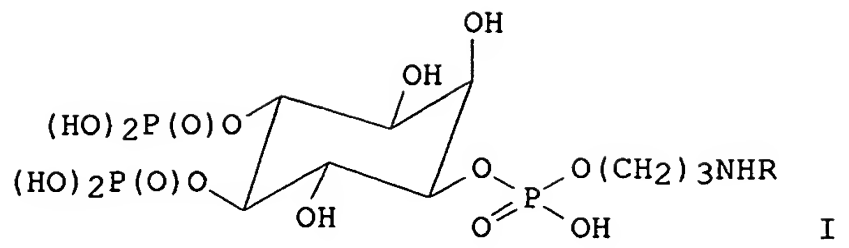
IT 135418-04-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of inositol tri- or tetraphosphate derivs.)
RN 135418-04-1 CAPLUS
CN myo-Inositol, 2-[4-amino-2-[(trifluoroacetyl)amino]benzoate]
1,4,5-tris(dihydrogen phosphate), monoammonium salt (9CI) (CA INDEX NAME)



● NH_3

L7 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:122884 CAPLUS
DOCUMENT NUMBER: 114:122884
TITLE: Tethered IP3. Synthesis and biochemical applications of the 1-O-(3-aminopropyl) ester of inositol (1,4,5)-trisphosphate
AUTHOR(S): Prestwich, Glenn D.; Marecek, James F.; Mourey, Robert J.; Theibert, Anne B.; Ferris, Christopher D.; Danoff, Sonye K.; Snyder, Solomon H.
CORPORATE SOURCE: Dep. Chem., State Univ. New York, Stony Brook, NY, 11794-3400, USA
SOURCE: Journal of the American Chemical Society (1991), 113(5), 1822-5
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:122884

GI



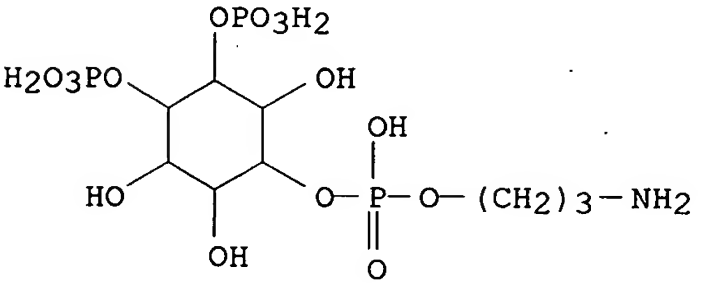
I

AB Phosphodiester analog I (R = H) of the second messenger Ins(1,4,5)P3 has been synthesized and used to prepare the novel photoaffinity label I [R = 4,2-N3(HO)C6H3CO] and the selective bioaffinity matrix I (R = affi-gel resin). A selectively protected inositol precursor was first converted by phosphite ester chemical to an N-protected 1-O-3-aminopropyl-1-phospho)-DL-myo-inositol and then phosphorylated to give a fully benzylated derivative Hydrogenolysis gives I (R = H). I all competed with [3H]Ins(1,4,5)P3 for binding to purified IP3 receptors from rat brain. Reconstituted receptor liposomes showed Ca release when stimulated by the tethered IP3 materials. None of the new materials were substrates for the 5-phosphatase or the 3-kinase that normally acts on Ins(1,4,5)P3.

IT 132071-99-9DP, polymer-bound 147852-81-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and interaction of, with inositol triphosphate receptor)

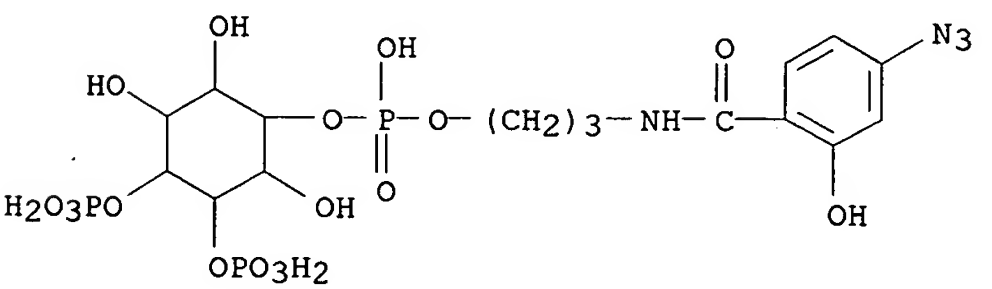
RN 132071-99-9 CAPLUS

CN myo-Inositol, 1-(3-aminopropyl hydrogen phosphate) 4,5-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)



RN 147852-81-1 CAPLUS

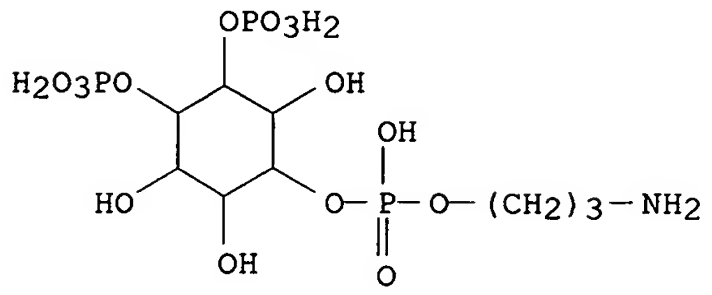
CN myo-Inositol, 1-[3-[(4-azido-2-hydroxybenzoyl)amino]propyl hydrogen phosphate] 4,5-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)



IT 132071-99-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with azidosalicylate)

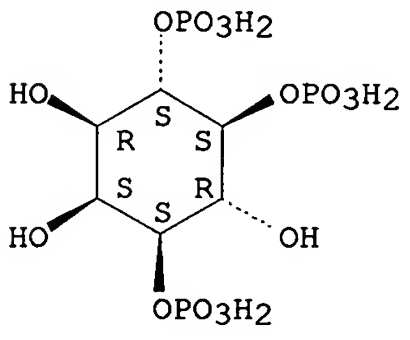
RN 132071-99-9 CAPLUS

CN myo-Inositol, 1-(3-aminopropyl hydrogen phosphate) 4,5-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

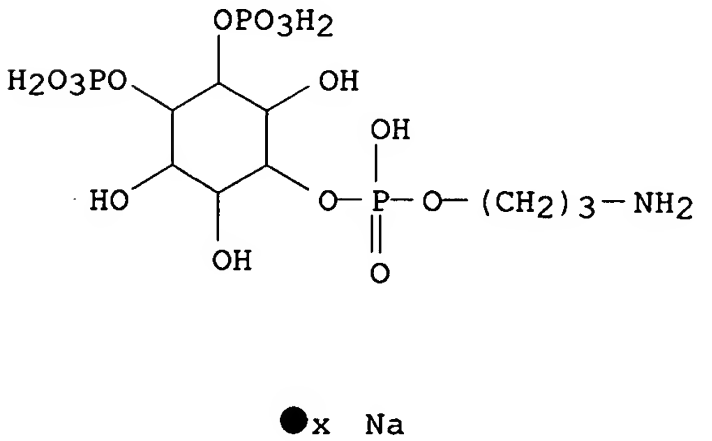


IT 88269-39-0DP, Inositol 1,4,5-triphosphate, analogs
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and receptor binding by)
RN 88269-39-0 CAPLUS
CN myo-Inositol, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 131932-42-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 131932-42-8 CAPLUS
CN myo-Inositol, 1-(3-aminopropyl hydrogen phosphate) 4,5-bis(dihydrogen phosphate), sodium salt (9CI) (CA INDEX NAME)




```
=> s IP3 conjugate
          5376 IP3
         67258 CONJUGATE
         60273 CONJUGATES
        104525 CONJUGATE
                (CONJUGATE OR CONJUGATES)
```

```
L8              0 IP3 CONJUGATE
                  (IP3(W)CONJUGATE)

=> s IP3 label
           5376 IP3
          63086 LABEL
          21921 LABELS
          75861 LABEL
                  (LABEL OR LABELS)
L9              0 IP3 LABEL
                  (IP3(W)LABEL)

=> s IP3 tracer
           5376 IP3
          54936 TRACER
          19021 TRACERS
          64953 TRACER
                  (TRACER OR TRACERS)
L10             0 IP3 TRACER
                  (IP3(W)TRACER)

=> s IP3 and competitive binding
           5376 IP3
          94907 COMPETITIVE
              5 COMPETITIVES
          94910 COMPETITIVE
                  (COMPETITIVE OR COMPETITIVES)
         955569 BINDING
           2080 BINDINGS
         956161 BINDING
                  (BINDING OR BINDINGS)
           5359 COMPETITIVE BINDING
                  (COMPETITIVE(W)BINDING)
L11            11 IP3 AND COMPETITIVE BINDING

=> s l11 and conjugate
          67258 CONJUGATE
          60273 CONJUGATES
         104525 CONJUGATE
                  (CONJUGATE OR CONJUGATES)
L12             0 L11 AND CONJUGATE

=> s l11 and label
          63086 LABEL
          21921 LABELS
          75861 LABEL
                  (LABEL OR LABELS)
L13             0 L11 AND LABEL

=> s IP3 assay and tracer
           5376 IP3
         365101 ASSAY
         160774 ASSAYS
         480953 ASSAY
                  (ASSAY OR ASSAYS)
              7 IP3 ASSAY
                  (IP3(W)ASSAY)
          54936 TRACER
          19021 TRACERS
          64953 TRACER
                  (TRACER OR TRACERS)
L14             0 IP3 ASSAY AND TRACER
```

```
=> s IP3 assay and conjugate
          5376 IP3
        365101 ASSAY
        160774 ASSAYS
        480953 ASSAY
                 (ASSAY OR ASSAYS)
             7 IP3 ASSAY
                 (IP3(W)ASSAY)
         67258 CONJUGATE
         60273 CONJUGATES
        104525 CONJUGATE
                 (CONJUGATE OR CONJUGATES)
L15          1 IP3 ASSAY AND CONJUGATE

=> s IP3 assay and label
          5376 IP3
        365101 ASSAY
        160774 ASSAYS
        480953 ASSAY
                 (ASSAY OR ASSAYS)
             7 IP3 ASSAY
                 (IP3(W)ASSAY)
         63086 LABEL
         21921 LABELS
         75861 LABEL
                 (LABEL OR LABELS)
L16          1 IP3 ASSAY AND LABEL

=> dup rem l15 l16
PROCESSING COMPLETED FOR L15
PROCESSING COMPLETED FOR L16
L17          1 DUP REM L15 L16 (1 DUPLICATE REMOVED)
               ANSWER '1' FROM FILE CAPLUS

=> d l1 ibib abs hitstr tot
L1 HAS NO ANSWERS
'IBIB ABS HITSTR ' IS NOT A VALID STRUCTURE FORMAT KEYWORD
Structure Formats
SIA ----- Structure Image, Attributes, and map table if it contains
          data.  (Default)
SIM ----- Structure IMage.
SAT ----- Structure ATtributes and map table if it contains data.
SCT ----- Structure Connection Table and map table if it contains
          data.
SDA ----- All Structure DAta (image, attributes, connection table and
          map table if it contains data).
NOS ----- NO Structure data.
ENTER STRUCTURE FORMAT (SIM), NOS:end

=> d l17 ibib abs hitstr tot

L17  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2007 ACS on STN  DUPLICATE 1
ACCESSION NUMBER:        2004:371146  CAPLUS
DOCUMENT NUMBER:         140:371475
TITLE:                   IP3 protein binding assay using detectably-labeled IP3
                         and an extracellular fragment of the IP3 receptor as
                         reagents
INVENTOR(S):             Naqvi, Tabassum; Rouhani, Riaz; Fung, Peter; Eglen,
                         Richard; Singh, Rajendra
PATENT ASSIGNEE(S):      Discoverx, Inc., USA
SOURCE:                  PCT Int. Appl., 38 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
```

Inventors

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004038369	A2	20040506	WO 2003-US33262	20031020
WO 2004038369	A3	20040701		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2503228	A1	20040506	CA 2003-2503228	20031020
AU 2003301583	A1	20040513	AU 2003-301583	20031020
US 2004106158	A1	20040603	US 2003-689122	20031020
EP 1556682	A2	20050727	EP 2003-809590	20031020
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006503582	T	20060202	JP 2004-546937	20031020
PRIORITY APPLN. INFO.:			US 2002-420469P P	20021021
			WO 2003-US33262 W	20031020

OTHER SOURCE(S): MARPAT 140:371475

AB Protein binding assays are provided for determining IP3 in a sample employing as

reagents a conjugate of IP3 joined at the 2-oxy through a bond or linking group to a detectable label and a truncated portion of the extracellular fragment of an IP3R. The reagents are combined with the sample and the amount of IP3 determined by means of the detectable label. The conjugate with the enzyme donor fragment of β-galactosidase or a fluorescer is specifically described.

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	143.83	316.14

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-11.70	-11.70

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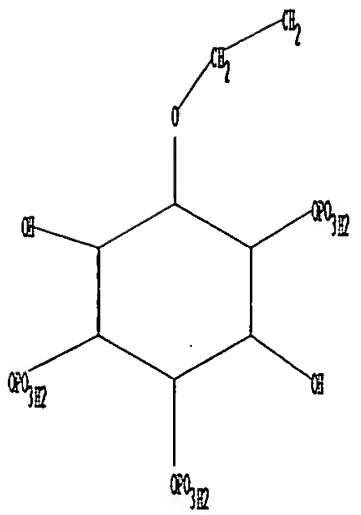

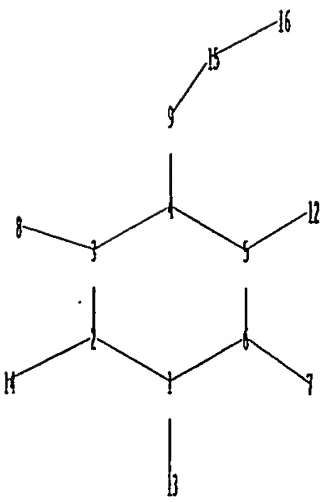

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ring nodes :
1 2 3 4 5 6
chain bonds :
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ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
3-8 4-9 6-7
exact bonds :
1-2 1-6 1-13 2-3 2-14 3-4 4-5 5-6 5-12 9-15 15-16
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS

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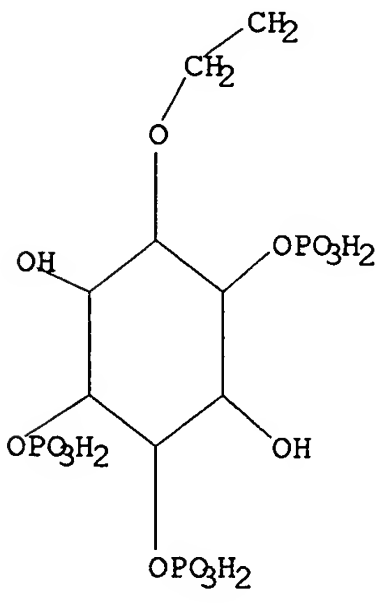

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED -       59 TO ITERATE

100.0% PROCESSED       59 ITERATIONS                                 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          720 TO     1640
PROJECTED ANSWERS:               2 TO      124

L2             2 SEA SSS SAM L1

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SEARCH TIME: 00.00.01

L3            20 SEA SSS FUL L1

=> FIL CAPLUS
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   172.10     172.31

FILE 'CAPLUS' ENTERED AT 17:46:11 ON 03 JAN 2007
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FILE COVERS 1907 - 3 Jan 2007  VOL 146 ISS 2
FILE LAST UPDATED: 2 Jan 2007  (20070102/ED)

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They are available for your review at:

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L4             7 L3

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L4   ANSWER 1 OF 7  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2004:371146  CAPLUS
DOCUMENT NUMBER:          140:371475
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TITLE: IP3 protein binding assay using detectably-labeled IP3 and an extracellular fragment of the IP3 receptor as reagents

INVENTOR(S): Naqvi, Tabassum; Rouhani, Riaz; Fung, Peter; Eglen, Richard; Singh, Rajendra

PATENT ASSIGNEE(S): Discoverx, Inc., USA

SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004038369	A2	20040506	WO 2003-US33262		20031020
WO 2004038369	A3	20040701			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2503228	A1	20040506	CA 2003-2503228		20031020
AU 2003301583	A1	20040513	AU 2003-301583		20031020
US 2004106158	A1	20040603	US 2003-689122		20031020
EP 1556682	A2	20050727	EP 2003-809590		20031020
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
JP 2006503582	T	20060202	JP 2004-546937		20031020

PRIORITY APPLN. INFO.:		
US 2002-420469P	P	20021021
WO 2003-US33262	W	20031020

OTHER SOURCE(S): MARPAT 140:371475

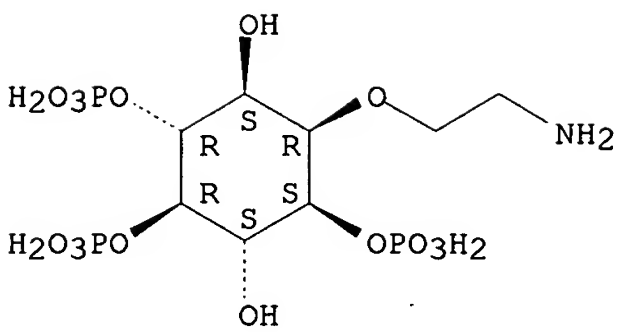
AB Protein binding assays are provided for determining IP3 in a sample employing as reagents a conjugate of IP3 joined at the 2-oxy through a bond or linking group to a detectable label and a truncated portion of the extracellular fragment of an IP3R. The reagents are combined with the sample and the amount of IP3 determined by means of the detectable label. The conjugate with the enzyme donor fragment of β-galactosidase or a fluorescer is specifically described.

IT 502159-32-2DP, reaction product with hexachlorofluorescein N-hydroxysuccinimide derivative 685515-03-1DP, conjugates with β-galactosidase fragment 685515-04-2P 685515-07-5P 685515-08-6P
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)
(IP3 protein binding assay using detectably-labeled IP3 and IP3 receptor extracellular fragment as reagents)

RN 502159-32-2 CAPLUS

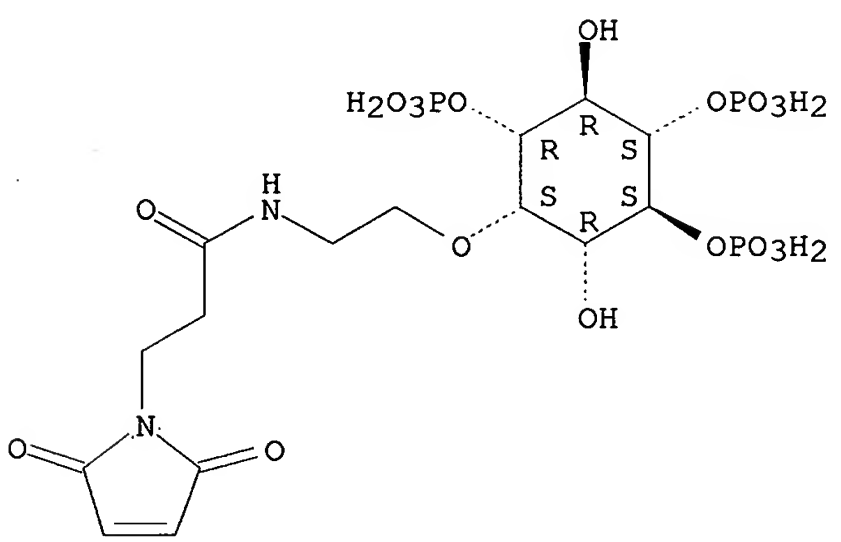
CN D-myo-Inositol, 2-O-(2-aminoethyl)-, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



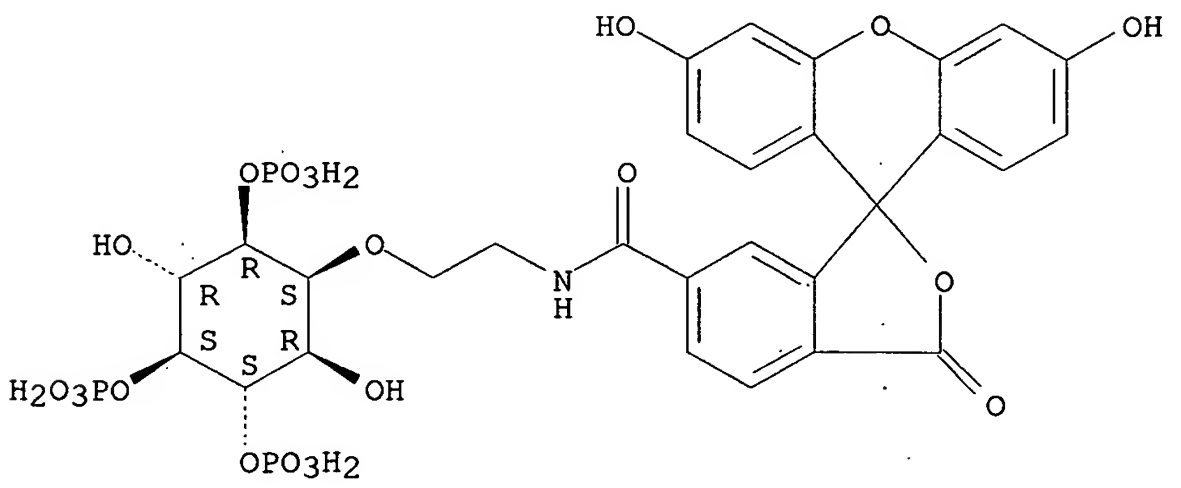
RN 685515-03-1 CAPLUS
CN D-myo-Inositol, 2-O-[2-[[3-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxopropyl]amino]ethyl]-, 3,5,6-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



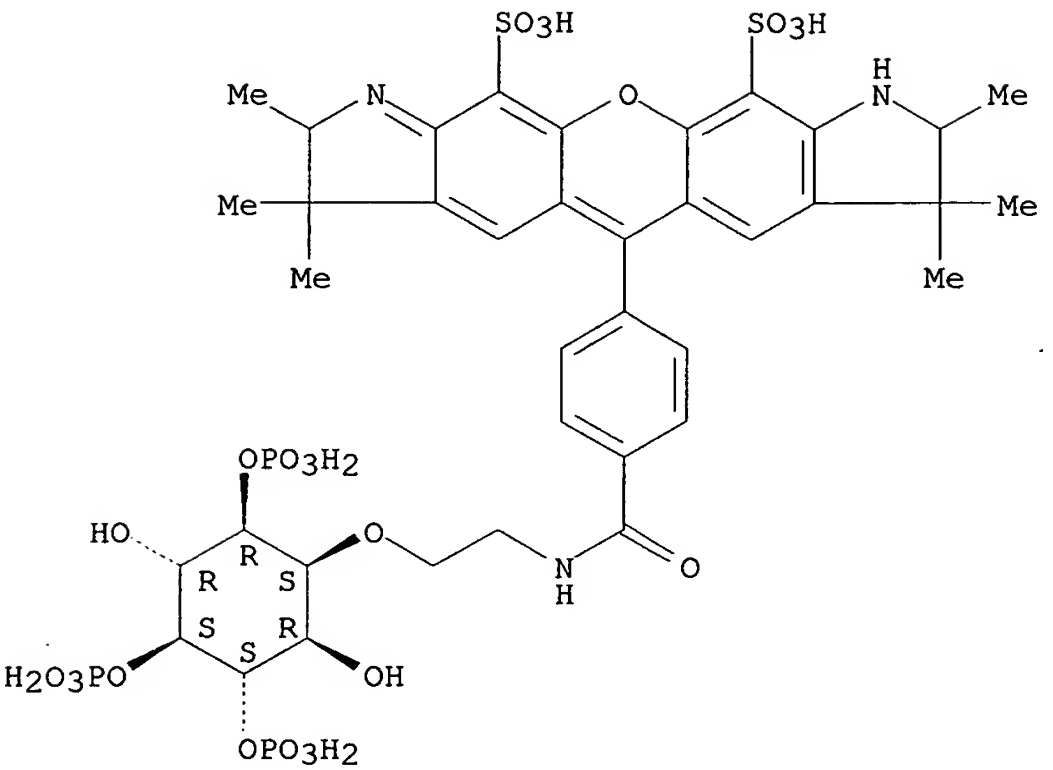
RN 685515-04-2 CAPLUS
CN D-myo-Inositol, 2-O-[2-[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl)carbonyl]amino]ethyl]-, 3,5,6-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 685515-07-5 CAPLUS
CN D-myo-Inositol, 2-O-[2-[[4-(2,3,7,8-tetrahydro-2,3,3,7,7,8-hexamethyl-10,12-disulfo-1H-pyrano[3,2-f:5,6-f']diindol-5-yl)benzoyl]amino]ethyl]-, 3,5,6-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

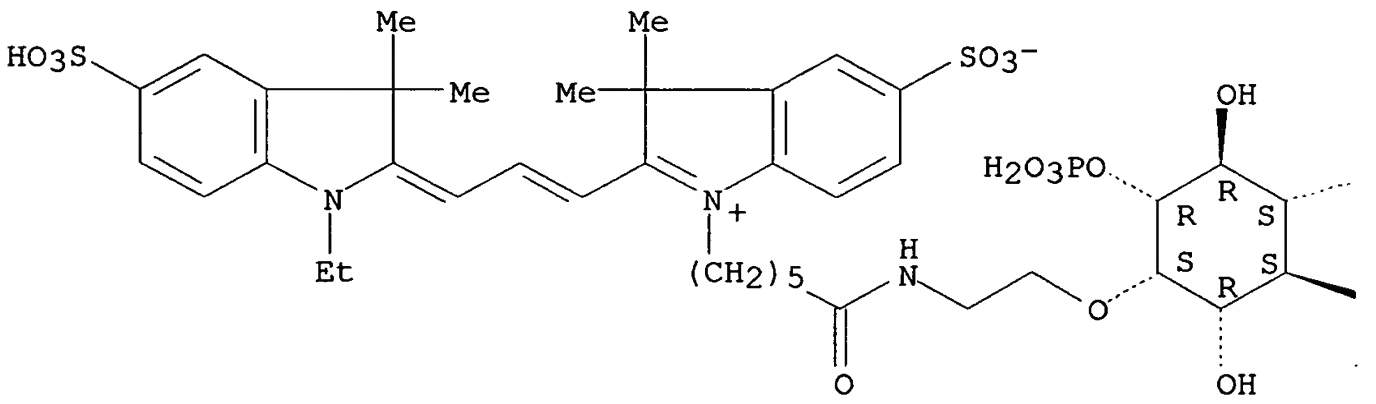
Absolute stereochemistry.



RN 685515-08-6 CAPLUS
CN D-myo-Inositol, 2-O-[2-[[6-[2-[3-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)-1-propenyl]-3,3-dimethyl-5-sulfo-3H-indolio]-1-oxohexyl]amino]ethyl]-, inner salt, 3,5,6-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



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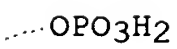
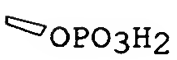




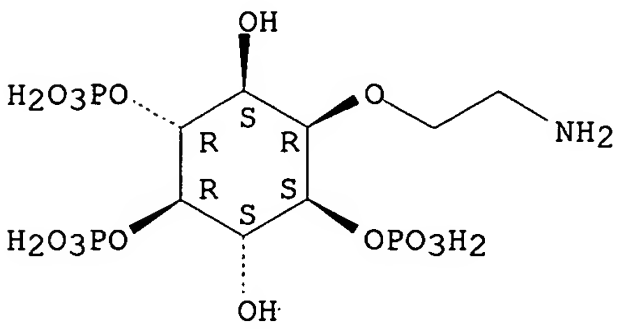
IT 502159-32-2 685515-06-4
RL: RCT (Reactant); RACT (Reactant or reagent)

(IP3 protein binding assay using detectably-labeled IP3 and IP3 receptor extracellular fragment as reagents)

RN 502159-32-2 CAPLUS

CN D-myo-Inositol, 2-O-(2-aminoethyl)-, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



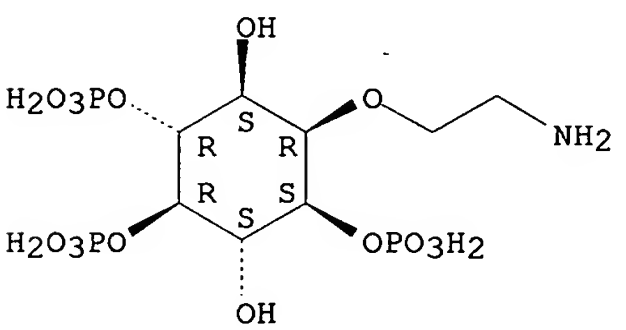
RN 685515-06-4 CAPLUS

CN D-myo-Inositol, 2-O-(2-aminoethyl)-, 1,4,5-tris(dihydrogen phosphate), compd. with N,N-diethylethanamine (9CI) (CA INDEX NAME)

CM 1

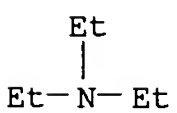
CRN 502159-32-2
CMF C8 H20 N O15 P3

Absolute stereochemistry.



CM 2

CRN 121-44-8
CMF C6 H15 N

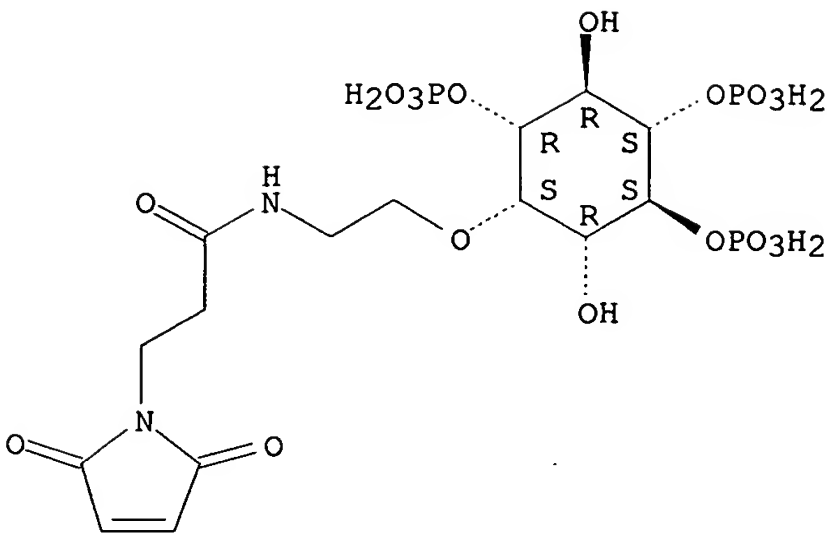


IT 685515-03-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(IP3 protein binding assay using detectably-labeled IP3 and IP3 receptor extracellular fragment as reagents)

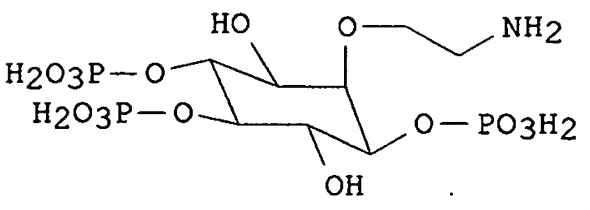
RN 685515-03-1 CAPLUS

CN D-myo-Inositol, 2-O-[2-[[3-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxopropyl]amino]ethyl]-, 3,5,6-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:364011 CAPLUS
DOCUMENT NUMBER: 141:123826
TITLE: 2-O-(2-Aminoethyl)-myo-inositol 1,4,5-trisphosphate as a novel ligand for conjugation: physicochemical properties and synthesis of a new Ins(1,4,5)P3 affinity matrix
AUTHOR(S): Riley, Andrew M.; Dozol, Helene; Spiess, Bernard; Potter, Barry V. L.
CORPORATE SOURCE: Department of Pharmacy and Pharmacology, Wolfson Laboratory of Medicinal Chemistry, University of Bath, Bath, BA2 7AY, UK
SOURCE: Biochemical and Biophysical Research Communications (2004), 318(2), 444-452
CODEN: BBRCA9; ISSN: 0006-291X
PUBLISHER: Elsevier Science
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:123826
GI



I

AB 2-O-(2-Aminoethyl)-Ins(1,4,5)P3 (I), a novel derivative of the Ca2+-mobilizing second messenger D-myo-inositol 1,4,5-trisphosphate [Ins(1,4,5)P3], was synthesized from myo-inositol. I was found to be a potent mobilizer of intracellular Ca2+, and an Ins(1,4,5)P3 affinity matrix synthesized from I was effective at selectively binding N-terminal fragments of the Ins(1,4,5)P3 receptor containing the intact Ins(1,4,5)P3 binding site. The micro-protonation scheme for I was resolved and the related consts. were determined in comparison with Ins(1,4,5)P3 and another reactive Ins(1,4,5)P3 analog 1-O-(2-aminoethyl-1-phospho)-Ins(4,5)P2 (II) by potentiometric and NMR titration methods. The 31P and 1H NMR titration curves for compound I and Ins(1,4,5)P3 are remarkably close, indicating analogous acid-base properties and intramol. interactions for the two compds. The 1-phosphate-modified Ins(1,4,5)P3 derivative II, on the contrary, behaves as a

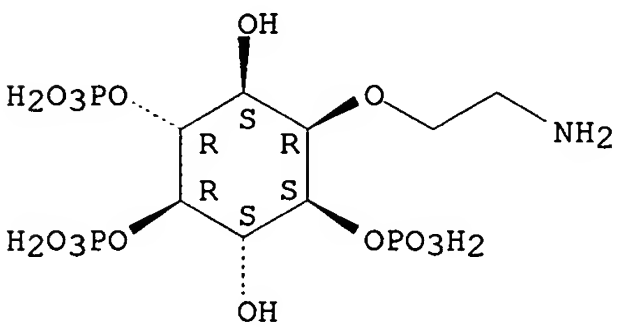
bis-phosphorylated rather than a tris-phosphorylated inositol. Thus, I is a new reactive Ins(1,4,5)P3 analog of considerable potential for investigation of the chemical biol. of Ins(1,4,5)P3-mediated cellular signaling.

IT 502159-32-2P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of aminoethyl-inositol trisphosphates as intracellular calcium ion mobilizer)

RN 502159-32-2 CAPLUS

CN D-myo-Inositol, 2-O-(2-aminoethyl)-, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:146720 CAPLUS

DOCUMENT NUMBER: 140:321602

TITLE: Dimers of D-myo-Inositol 1,4,5-Trisphosphate: Design, Synthesis, and Interaction with Ins(1,4,5)P3 Receptors

AUTHOR(S): Riley, Andrew M.; Laude, Alex J.; Taylor, Colin W.; Potter, Barry V. L.

CORPORATE SOURCE: Wolfson Laboratory of Medicinal Chemistry, Department of Pharmacy and Pharmacology, University of Bath, Bath, BA2 7AY, UK

SOURCE: Bioconjugate Chemistry (2004), 15(2), 278-289
CODEN: BCCHES; ISSN: 1043-1802

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:321602

AB The design and synthesis of dimeric versions of the intracellular signaling mol. D-myo-inositol 1,4,5-trisphosphate [Ins(1,4,5)P3] are reported. Ins(1,4,5)P3 dimers in a range of sizes were constructed by conjugation of a partially protected 2-O-(2-aminoethyl)-Ins(1,4,5)P3 intermediate with activated oligo- and poly(ethylene glycol) (PEG) tethers, to give benzyl-protected dimers with amide or carbamate linkages. After deprotection, the resulting water-soluble Ins(1,4,5)P3 dimers were purified by ion-exchange chromatog. The interaction of the Ins(1,4,5)P3 dimers with tetrameric Ins(1,4,5)P3 receptors was explored, using equilibrium [3H]Ins(1,4,5)P3-binding to membranes from cerebellum, and 45Ca2+-release from permeabilized hepatocytes. The results showed that dimers, even when they incorporate large PEG tethers, interact potently with Ins(1,4,5)P3 receptors, and that the shorter dimers are more potent than Ins(1,4,5)P3 itself. A very small dimer, consisting of two Ins(1,4,5)P3 motifs joined by a short N,N'-diethylurea spacer, was synthesized. Preliminary studies of 45Ca2+ release from the intracellular stores of permeabilized hepatocytes showed this shortest dimer to be almost as potent as adenophostin A, the most potent Ins(1,4,5)P3 receptor ligand known.

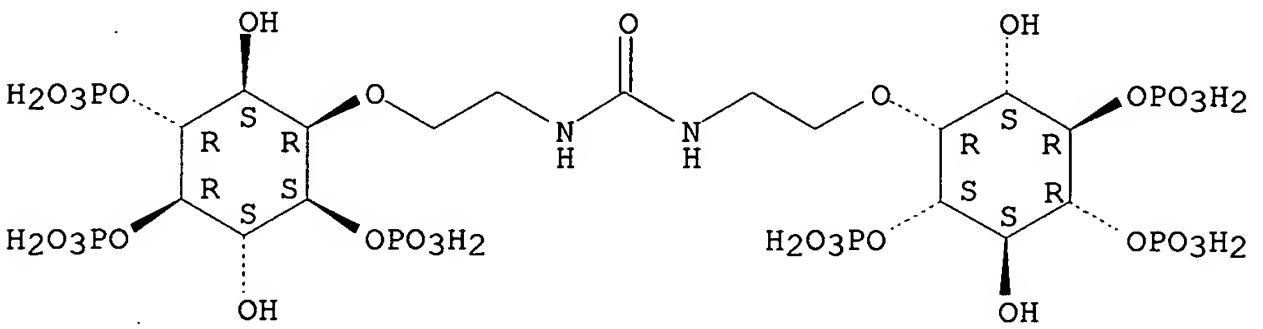
Possible interpretations of this result are considered in relation to the recently disclosed x-ray crystal structure of the type 1 Ins(1,4,5)P3 receptor core binding domain.

IT 678150-59-9P
RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(crystal structure; design and synthesis of inositol trisphosphate and interaction with Ins(1,4,5)P3 receptors)

RN 678150-59-9 CAPLUS

CN D-myo-Inositol, 2,2'-O-[carbonylbis(imino-2,1-ethanediyl)]bis-, 1,1',4,4',5,5'-hexakis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



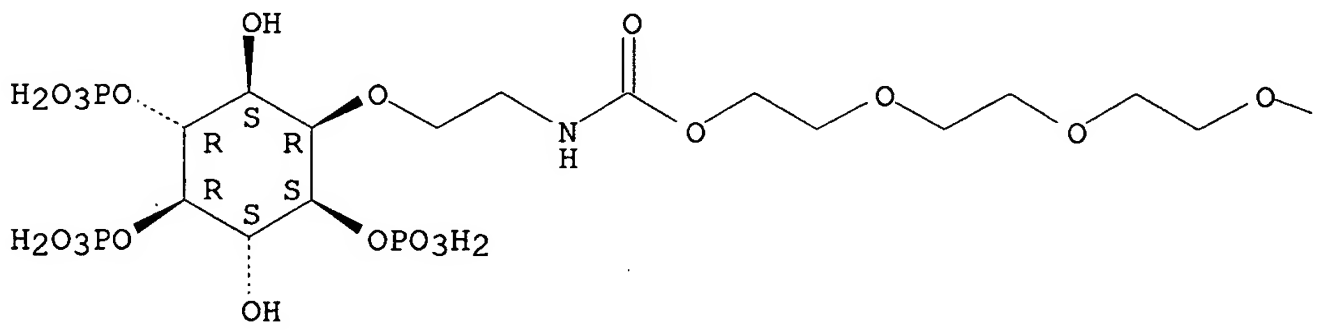
IT 288861-59-6P 288861-60-9P 502159-30-0P
502159-33-3P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(design and synthesis of inositol trisphosphate and interaction with Ins(1,4,5)P3 receptors)

RN 288861-59-6 CAPLUS

CN D-myo-Inositol, 2,2'-O-(4,24-dioxo-5,8,11,14,17,20,23-heptaoxa-3,25-diazaheptacosane-1,27-diyl)bis-, 1,1',4,4',5,5'-hexakis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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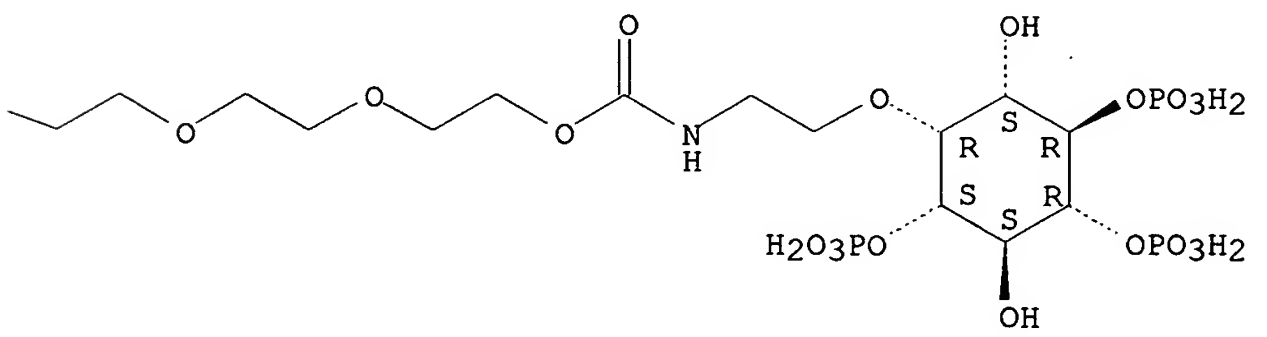
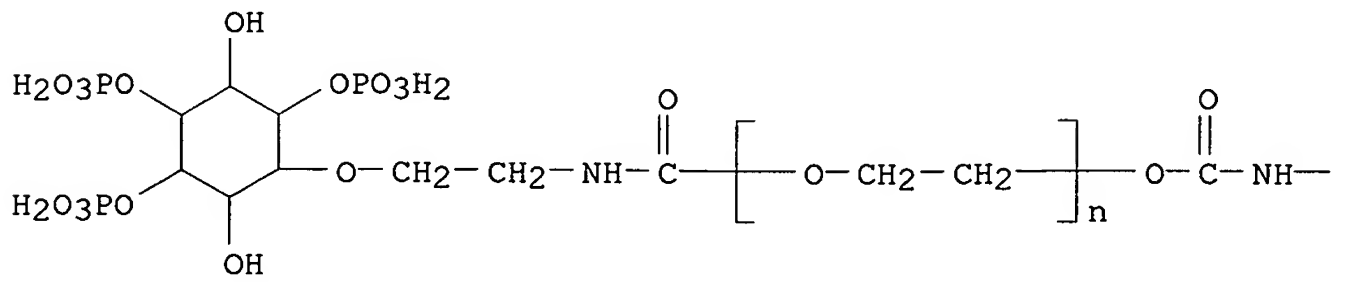


RN 288861-60-9 CAPLUS
CN Poly(oxy-1,2-ethanediyl), α-hydro-ω-hydroxy-, diester with 2-O-[2-(carboxyamino)ethyl]-D-myo-inositol 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

PAGE 1-A



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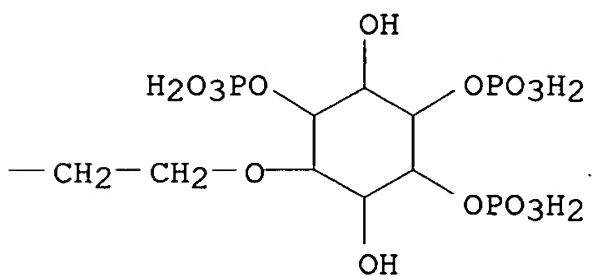
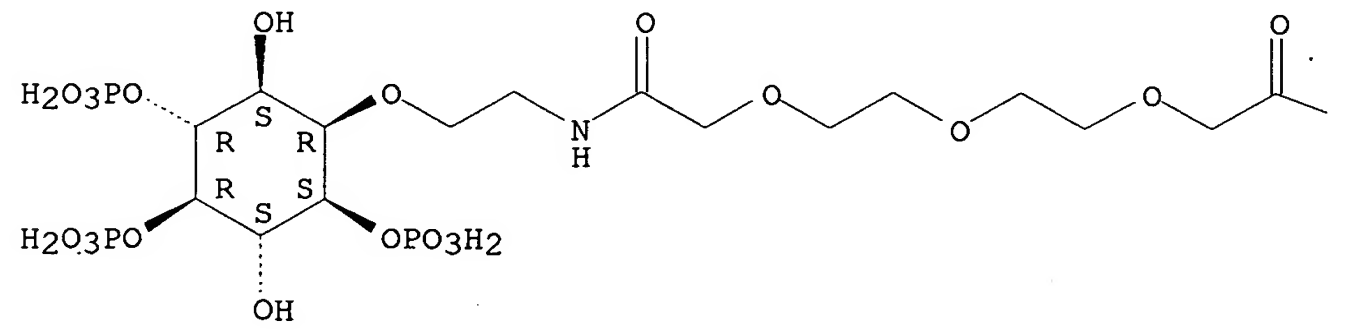


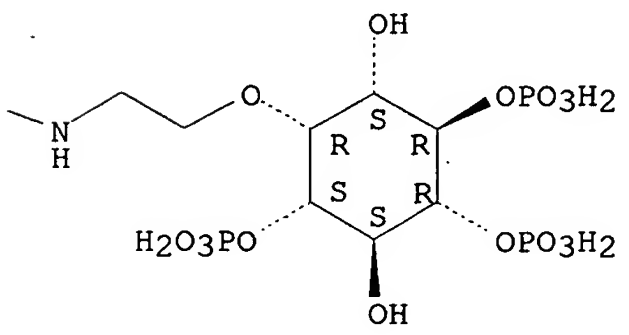
RN 502159-30-0 CAPLUS
CN D-myo-Inositol, 2,2'-O-(4,14-dioxo-6,9,12-trioxa-3,15-diazaheptadecane-1,17-diyl)bis-, 1,1',4,4',5,5'-hexakis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 1-B

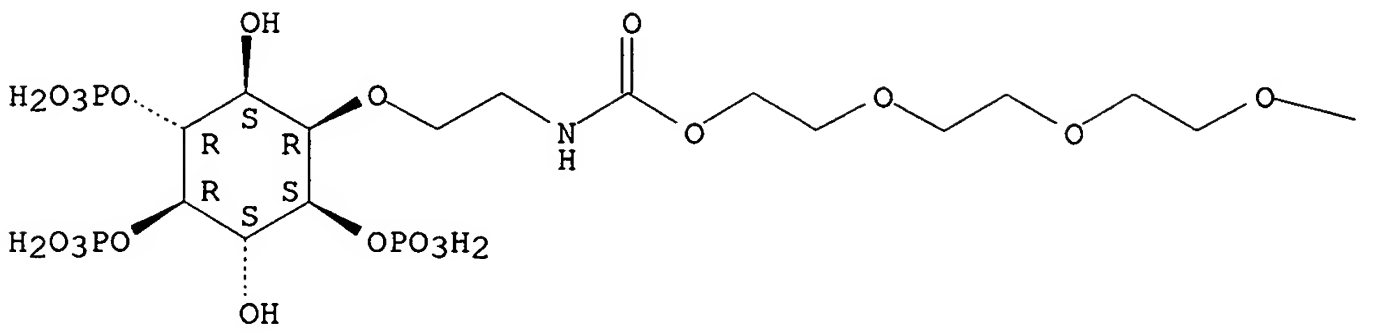


RN 502159-33-3 CAPLUS
CN D-myo-Inositol, 2-O-(4-oxo-5,8,11,14,17,20,23-heptaoxa-3-azatetracos-1-yl)-

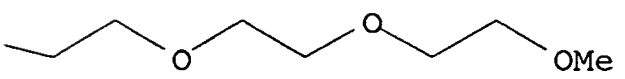
, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:946809 CAPLUS
DOCUMENT NUMBER: 140:235954
TITLE: First derivatives of myo-inositol 1,4,6-trisphosphate modified at positions 2 and 3: structural analogues of D-myo-inositol 1,4,5-trisphosphate
AUTHOR(S): Horne, Graeme; Mills, Stephen J.; Potter, Barry V. L.
CORPORATE SOURCE: Department of Pharmacy and Pharmacology, Wolfson Laboratory of Medicinal Chemistry, University of Bath, Bath, BA2 7AY, UK
SOURCE: Carbohydrate Research (2004), 339(1), 51-65
CODEN: CRBRAT; ISSN: 0008-6215
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:235954

AB Novel, structurally modified potential mimics of the second messenger D-myo-inositol 1,4,5-trisphosphate, based on the biol. active regioisomer D-myo-inositol 1,4,6-trisphosphate, were synthesized. DL-5-O-Benzyl-1,4,6-tri-O-p-methoxybenzyl-myo-inositol was the key intermediate for the preparation of the following compds.: DL-3-deoxy-, DL-3-deoxy-2-O-methyl-, DL-3-O-(2-hydroxyethyl)-, DL-3-O-(3-hydroxypropyl)- and DL-3-O-(4-hydroxybutyl)-myo-inositol 1,4,6-trisphosphate. DL-1,4,6-Tri-O-allyl-5-O-benzyl-myo-inositol was used to prepare DL-2-O-methyl-myo-inositol 1,4,6-trisphosphate. Deoxy-compds. were prepared by reduction of the corresponding tosylated intermediate using Super Hydride. The hydroxyalkyl groups were introduced at the C-3 of myo-inositol using the corresponding benzyl protected hydroxy alkyl bromide via the cis-2,3-O-dibutylstannylene acetal. Methylation and benzylation at C-2 was accomplished using Me iodide and benzyl bromide, resp., in the presence of sodium hydride. Deblocking of p-methoxybenzyl groups was accomplished with TFA in dichloromethane and the allyl groups were removed by isomerization to the cis-prop-1-enyl derivative, which was hydrolyzed under acidic conditions to give the corresponding 1,4,6-triol. The 1,4,6-triols were phosphitylated with the P(III) reagent bis(benzyloxy)(diisopropylamin o)phosphine in the presence of 1H-tetrazole then oxidized with

3-chloroperoxybenzoic acid followed by deblocking by hydrogenolysis to give DL-2-O-methyl-, DL-3-O-deoxy-, DL-3-O-deoxy-2-O-methyl-, DL-3-O-(2-hydroxyethyl)-, DL-3-O-(3-hydroxypropyl)- and DL-3-O-(4-hydroxybutyl)-myo-inositol 1,4,6-trisphosphate, resp.

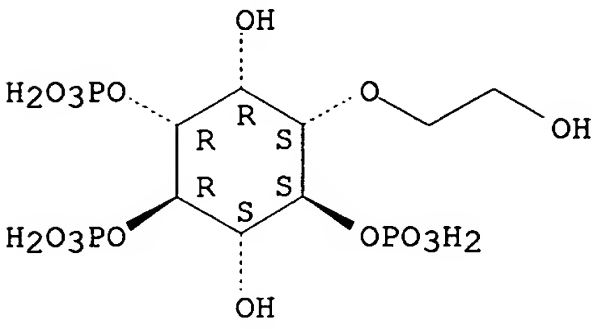
IT 860304-99-0P 860305-18-6P 860305-44-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2-O and 3-O modified myo-inositol 1,4,6-trisphosphate derivs.)

RN 860304-99-0 CAPLUS
CN myo-Inositol, 1-O-(2-hydroxyethyl)-, 3,4,6-tris(dihydrogen phosphate), compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

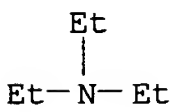
CRN 666835-05-8
CMF C8 H19 O16 P3

Relative stereochemistry.



CM 2

CRN 121-44-8
CMF C6 H15 N

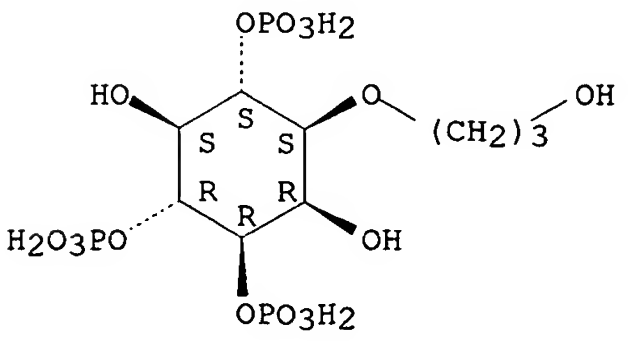


RN 860305-18-6 CAPLUS
CN myo-Inositol, 1-O-(3-hydroxypropyl)-, 3,4,6-tris(dihydrogen phosphate), compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

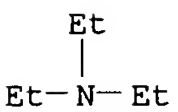
CRN 666835-06-9
CMF C9 H21 O16 P3

Relative stereochemistry.



CM 2

CRN 121-44-8
CMF C6 H15 N

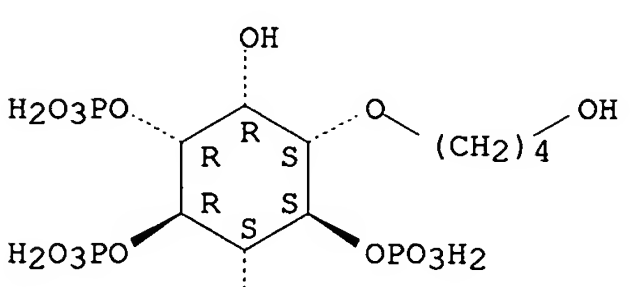


RN 860305-44-8 CAPLUS
CN myo-Inositol, 1-O-(4-hydroxybutyl)-, 3,4,6-tris(dihydrogen phosphate), compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

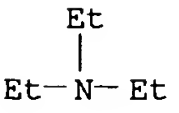
CRN 666835-07-0
CMF C10 H23 O16 P3

Relative stereochemistry.



CM 2

CRN 121-44-8
CMF C6 H15 N



REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:798417 CAPLUS
DOCUMENT NUMBER: 138:250343
TITLE: Interactions of Inositol 1,4,5-Trisphosphate (IP3) Receptors with Synthetic Poly(ethylene glycol)-linked Dimers of IP3 Suggest Close Spacing of the IP3-binding Sites
AUTHOR(S): Riley, Andrew M.; Morris, Stephen A.; Nerou, Edmund P.; Correa, Vanessa; Potter, Barry V. L.; Taylor, Colin W.
CORPORATE SOURCE: Department of Pharmacy and Pharmacology, Wolfson Laboratory of Medicinal Chemistry, University of Bath, Claverton Down, Bath, BA2 7AY, UK

SOURCE: Journal of Biological Chemistry (2002), 277(43), 40290-40295
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

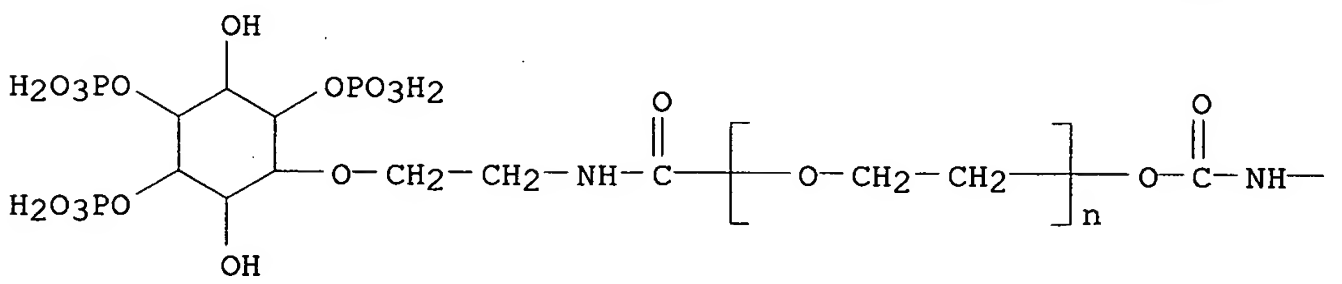
AB The distances between the inositol 1,4,5-trisphosphate (IP3)-binding sites of tetrameric IP3 receptors were probed using dimers of IP3 linked by poly(ethylene glycol) (PEG) mols. of differing lengths (1-8 nm). Each of the dimers potently stimulated 45Ca2+ release from permeabilized cells expressing predominantly type 1 (SH-SY5Y cells) or type 2 (hepatocytes) IP3 receptors. The shortest dimers, with PEG linkers of an effective length of 1.5 nm or less, were the most potent, being 3-4-fold more potent than IP3. In radioligand binding expts. using cerebellar membranes, the shortest dimers bound with highest affinity, although the longest dimer (8 nm) also bound with almost 4-fold greater affinity than IP3. The affinity of monomeric IP3 with only the PEG attached was 2-fold weaker than IP3, confirming that the increased affinity of the dimers requires the presence of both IP3 motifs. The increased affinity of the long dimer probably results from the linked IP3 mols. binding to sites on different receptors, because the dimer bound with greater affinity than IP3 to cerebellar membranes, where receptors are densely packed, but with the same affinity as IP3 to purified receptors. IP3 and the IP3 dimers, irresp. of their length, bound with similar affinity to a monomeric IP3-binding domain of the type 1 IP3 receptor expressed in bacteria. Short dimers therefore bind with increased affinity only when the receptor is tetrameric. We conclude that the four IP3-binding sites of an IP3 receptor may be separated by as little as 1.5 nm and are therefore likely to be placed centrally in this large (25 + 25 nm) structure, consistent with previous work indicating a close association between the central pore and the IP3-binding sites of the IP3 receptor.

IT 288861-60-9P 502159-30-0P 502159-31-1P
502159-32-2P 502159-33-3P
RL: BSU (Biological study, unclassified); PNU (Preparation, unclassified); BIOL (Biological study); PREP (Preparation)
(interactions of tetrameric IP3 receptors with synthetic PEG-linked dimers of IP3 suggest close spacing of IP3-binding sites)

RN 288861-60-9 CAPLUS

CN Poly(oxy-1,2-ethanediyl), α-hydro-ω-hydroxy-, diester with 2-O-[2-(carboxyamino)ethyl]-D-myo-inositol 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

PAGE 1-A



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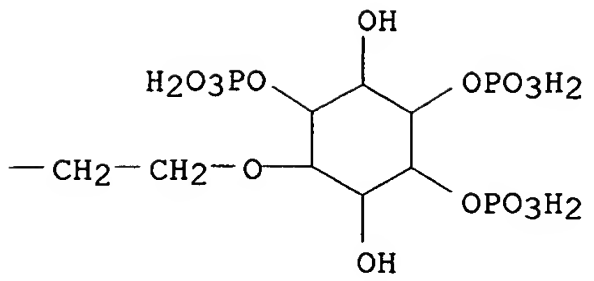
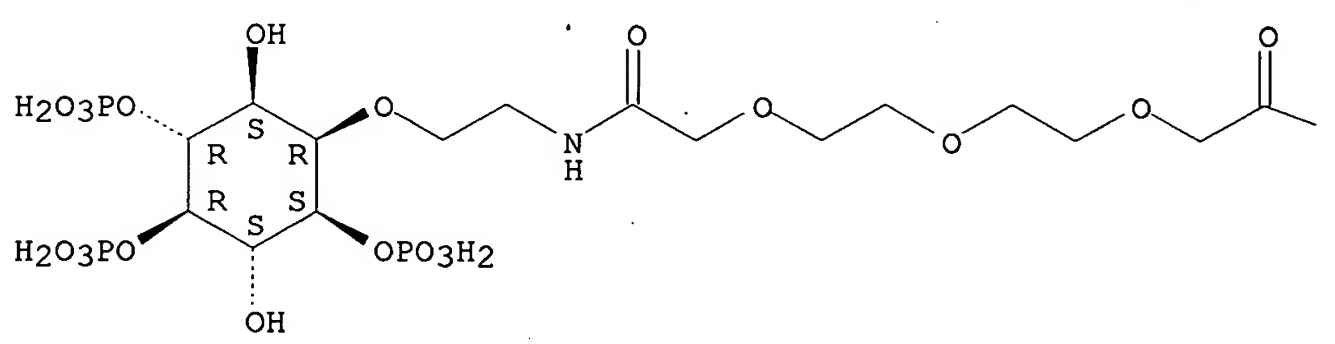


RN 502159-30-0 CAPLUS
CN D-myo-Inositol, 2,2'-O-(4,14-dioxo-6,9,12-trioxa-3,15-diazaheptadecane-1,17-diyl)bis-, 1,1',4,4',5,5'-hexakis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



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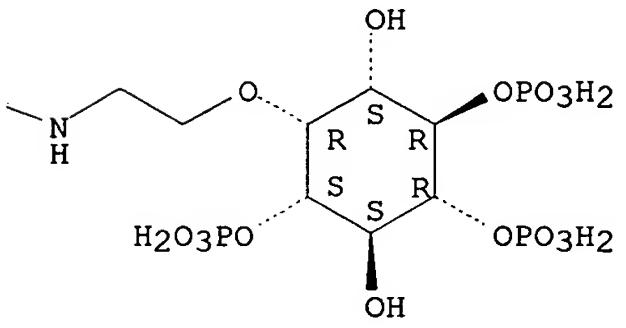
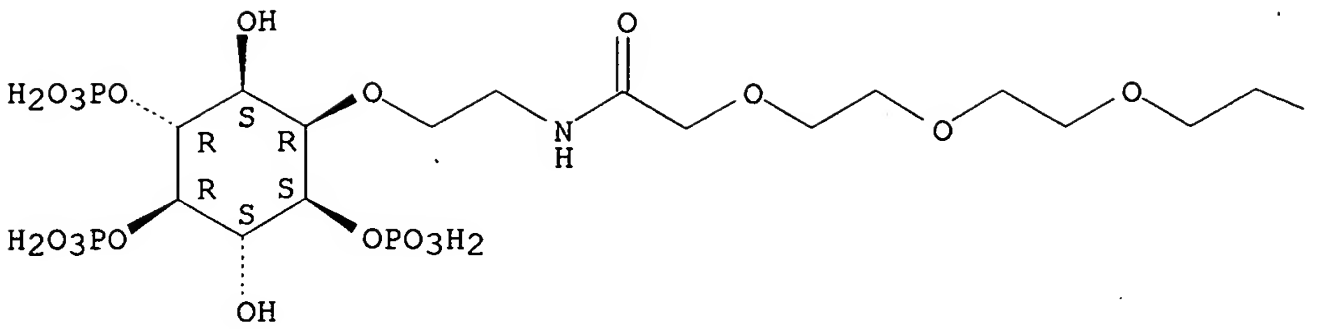


RN 502159-31-1 CAPLUS
CN D-myo-Inositol, 2,2'-O-(4,41-dioxo-6,9,12,15,18,21,24,27,30,33,36,39-dodecaoxa-3,42-diazatetratetracontane-1,44-diyl)bis-, 1,1',4,4',5,5'-hexakis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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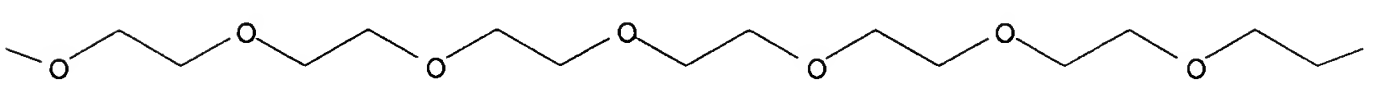

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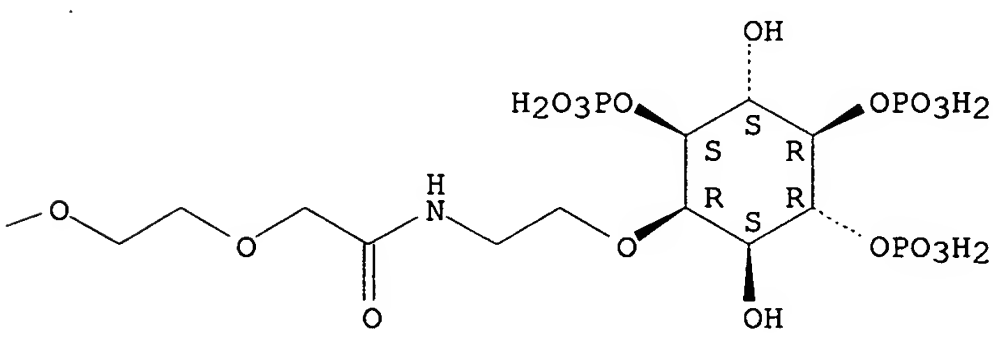
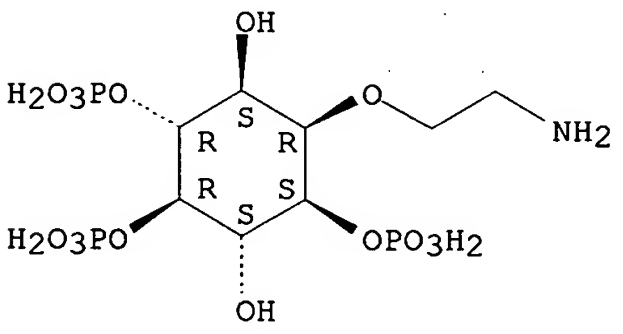


RN 502159-32-2 CAPLUS
CN D-myo-Inositol, 2-O-(2-aminoethyl)-, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

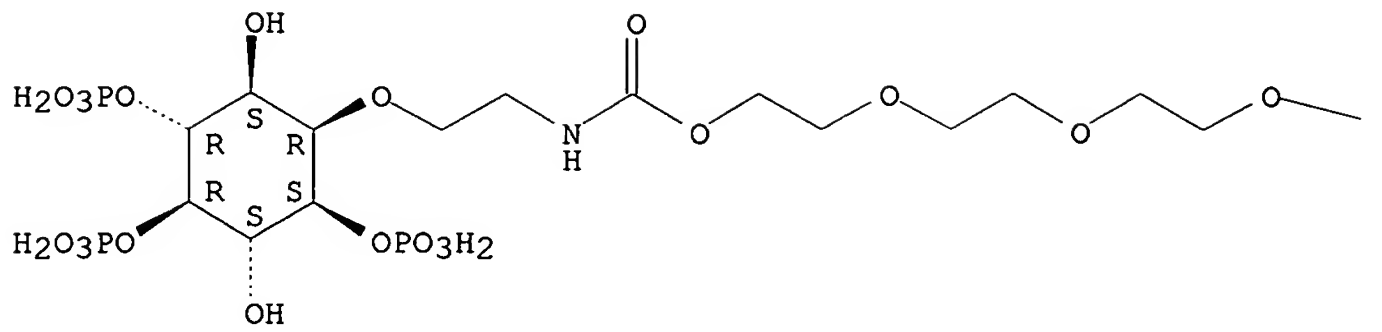
Absolute stereochemistry.



RN 502159-33-3 CAPLUS
CN D-myo-Inositol, 2-O-(4-oxo-5,8,11,14,17,20,23-heptaoxa-3-azatetracos-1-yl)-, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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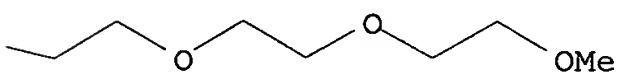
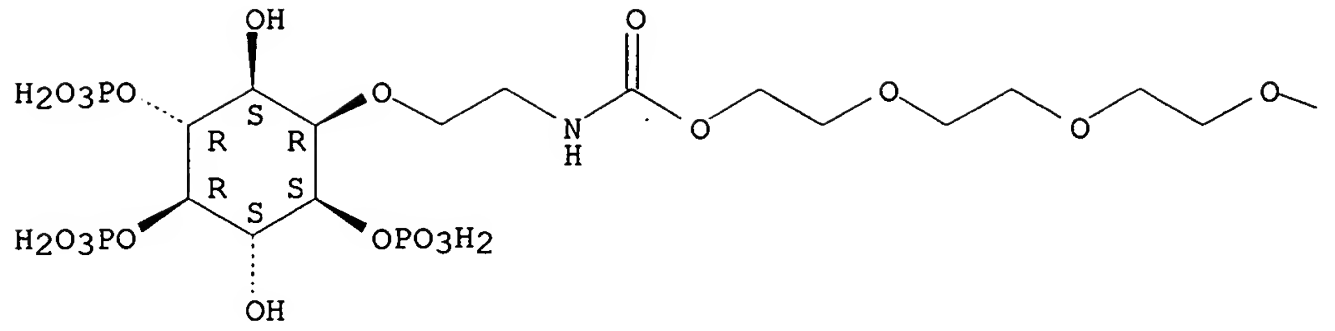


REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:350708 CAPLUS
DOCUMENT NUMBER: 133:193370
TITLE: Poly(ethylene glycol)-linked dimers of D-myo-inositol 1,4,5-trisphosphate
AUTHOR(S): Riley, Andrew M.; Potter, Barry V. L.
CORPORATE SOURCE: Wolfson Lab. Med. Chem., Dep. Pharm. Pharmacol., University of Bath, Bath, BA2 7AY, UK
SOURCE: Chemical Communications (Cambridge) (2000), (11), 983-984
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The first poly(ethylene glycol)-linked dimers of d-myo-inositol 1,4,5-trisphosphate have been synthesized as probes for multi-subunit binding proteins of this ubiquitous second messenger.
IT 288861-59-6P 288861-60-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of poly(ethylene glycol)-linked dimers of D-inositol 1,4,5-trisphosphate)
RN 288861-59-6 CAPLUS
CN D-myo-Inositol, 2,2'-O-(4,24-dioxo-5,8,11,14,17,20,23-heptaoxa-3,25-diazaheptacosane-1,27-diyl)bis-, 1,1',4,4',5,5'-hexakis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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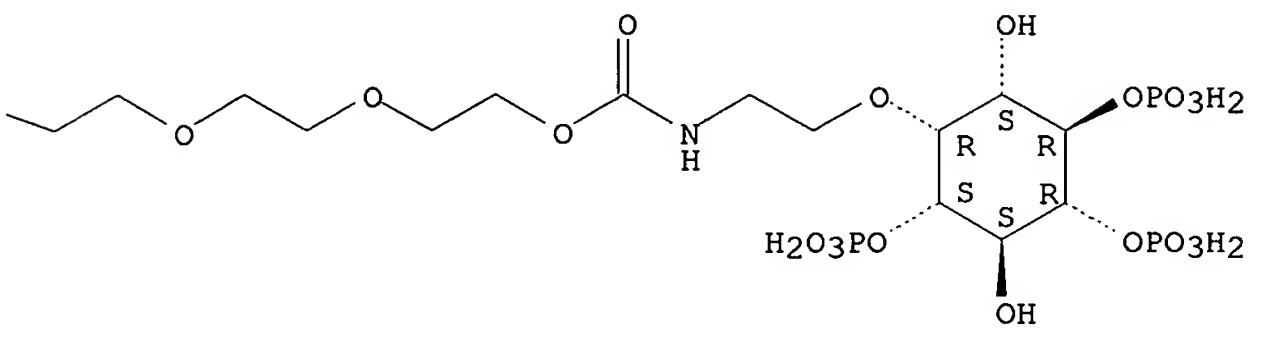
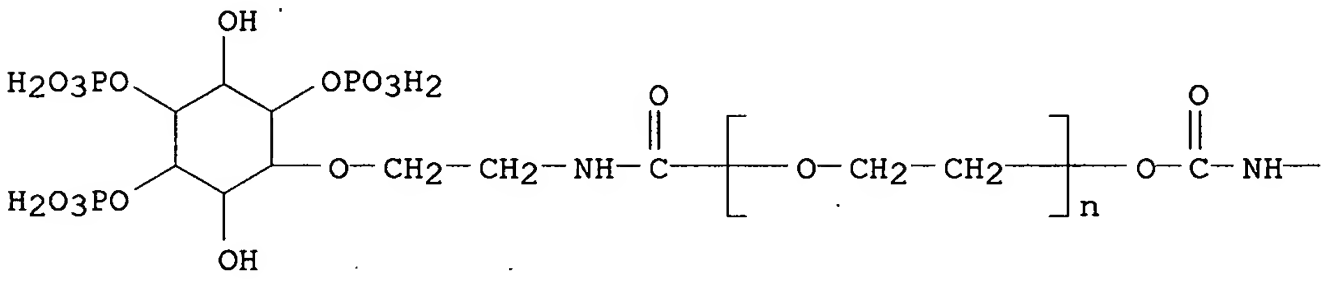


RN 288861-60-9 CAPLUS
CN Poly(oxy-1,2-ethanediyl), α-hydro-ω-hydroxy-, diester with 2-O-[2-(carboxyamino)ethyl]-D-myo-inositol 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)

PAGE 1-A



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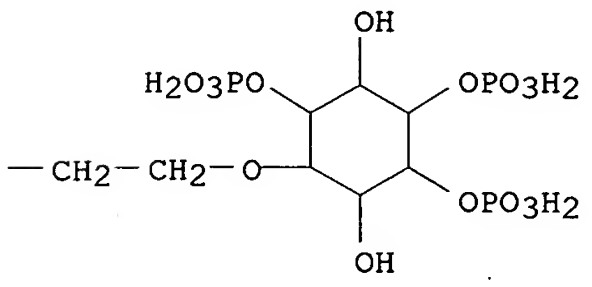


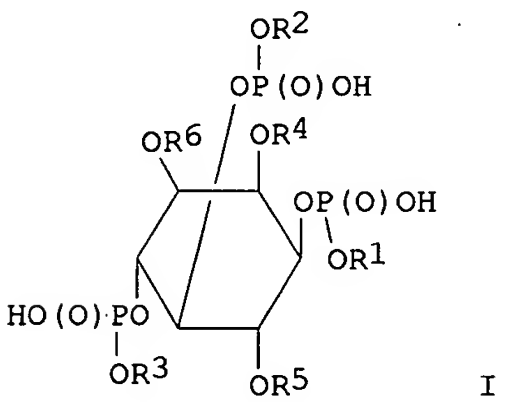
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:525262 CAPLUS
DOCUMENT NUMBER: 121:125262
TITLE: preparation of myo-inositol derivatives as cell activators

INVENTOR(S): Mikoshiba, Katsuhiko; Ozaki, Shoichiro
PATENT ASSIGNEE(S): Soosei Kk, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06135835	A	19940517	JP 1992-313956	19921028

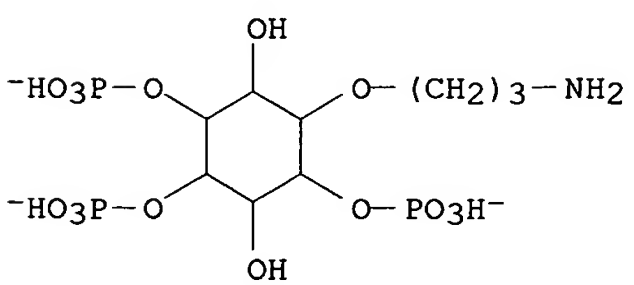
PRIORITY APPLN. INFO.: JP 1992-313956 19921028
OTHER SOURCE(S): MARPAT 121:125262
GI



I

AB Myoinositol derivs. (I)[R1-3 = H, lower alkyl; R4-6 = H, lower alkyl, aminoalkyl, lower alkanoyl; R1 = R2 = R3 = R4= R5= R6 ≠ H] are cell activators. I stimulated the release of calcium from receptors and, as a result , activated cells. I improved e.g. the lowered hormone secretion and brain function and are useful in treating smooth muscle dysfunction-related diseases (no data). D-2,3,6-tribenzylmyoinositol in THF was sirred with dibutylbenzylpyrophosphoric acid and Bu lithium and then with ammonium acetate to give D-1,4,5-tris(butylphospho)myoinositol triammonium salt (II). II promoted the release of calcium from A10 cells. II 1, mannitol 1g, sorbitol 80 10mg, and saline 100 mL were mixed, distributed into vials, and freeze-dried to give an injection.

IT 157067-94-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, for preparing myoinositol derivs. as cell activators)
RN 157067-94-2 CAPLUS
CN D-myo-Inositol, 2-O-(3-aminopropyl)-, 1,4,5-tris(dihydrogen phosphate) (9CI) (CA INDEX NAME)



IT 157067-95-3P